PROCESS MODELING

COURSE for 2nd year,

Automation and Applied Informatics,

TUCN

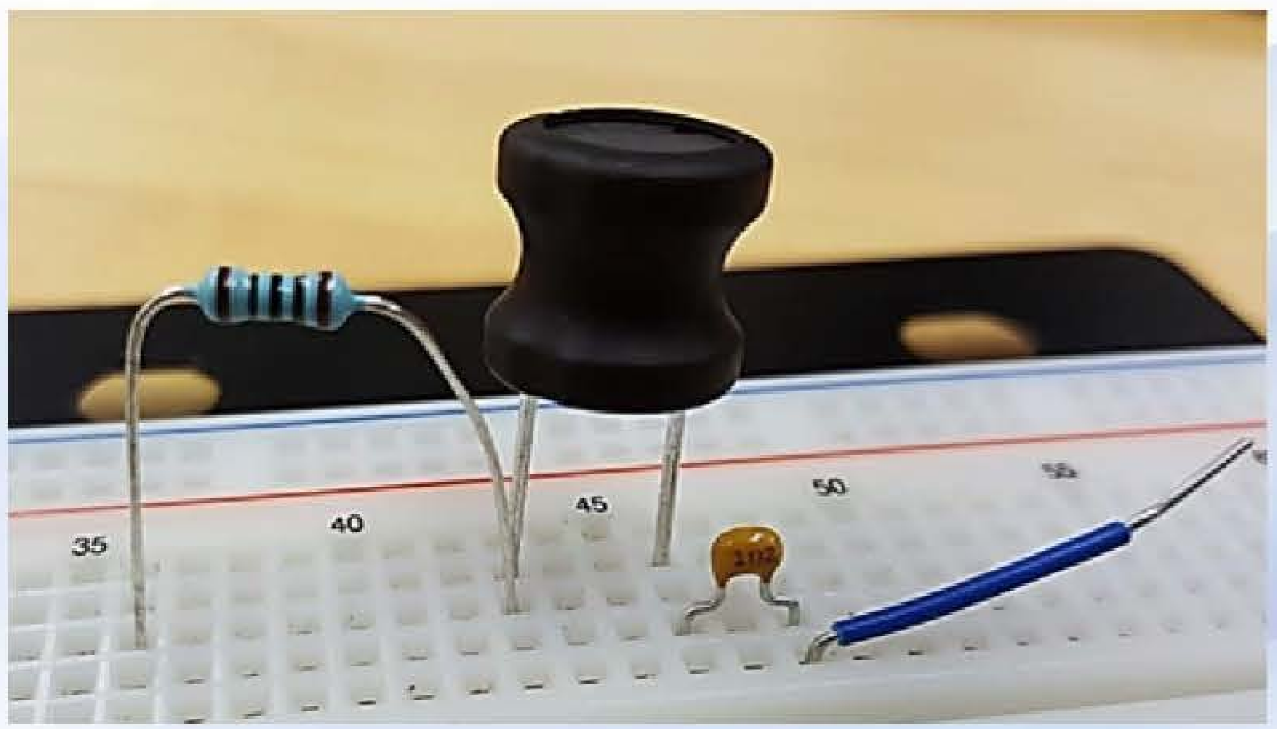
- Models take a central position in all process engineering tasks as they replace the process for the analysis.

They represent ***an abstraction of the process***, NOT *a complete reproduction*. Models make it possible to study the behavior of a process within the domain of common characteristics of the model and the modeled process <u>without affecting the original process</u>.

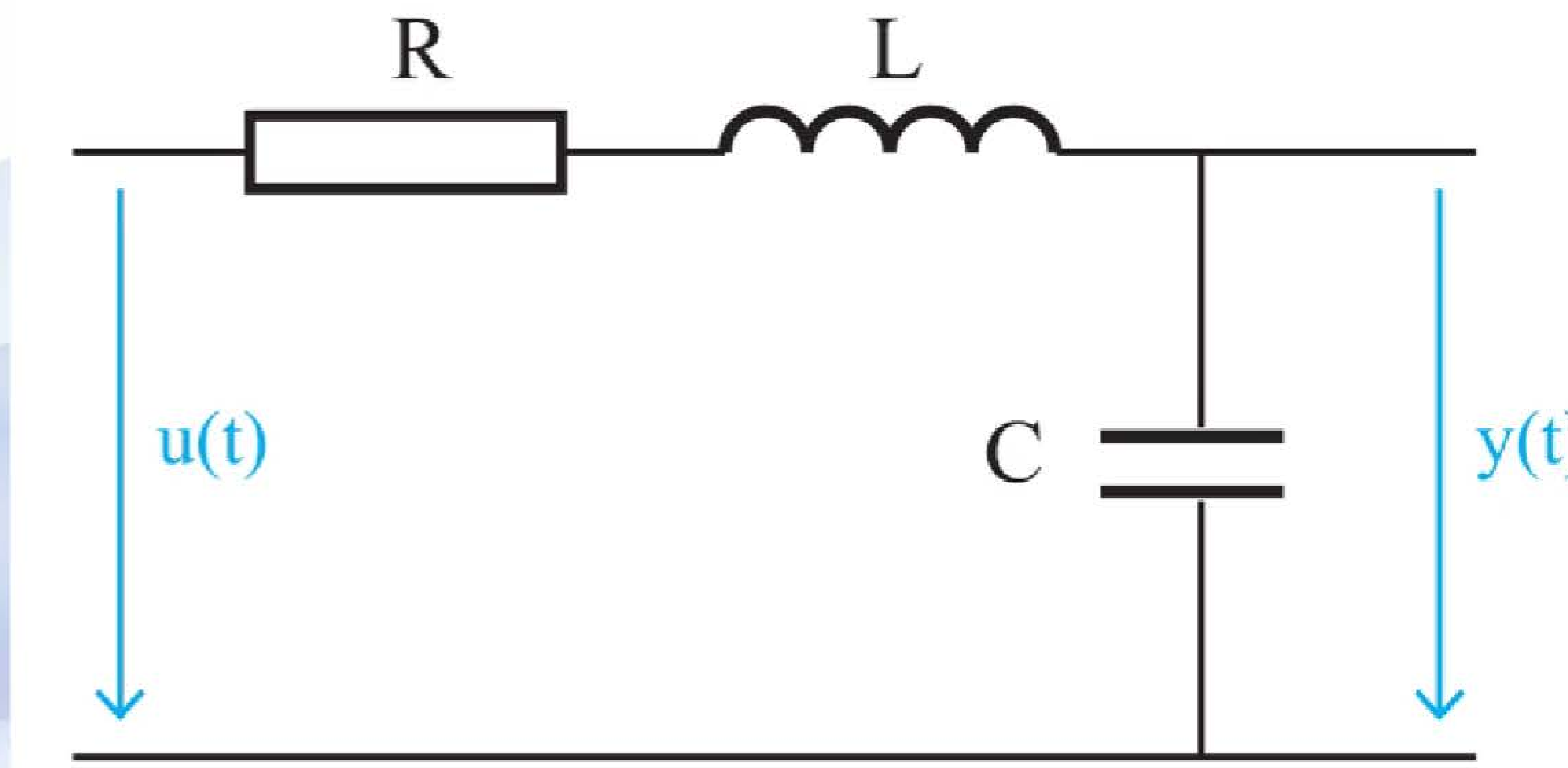
Models have a vast variety of applications in:

- measurement methods,
- design of experiments,
- product design and development,
- industrial process control,
- public health programmes,
- economic planning

Example: the real system and the model represented as a schematic diagram



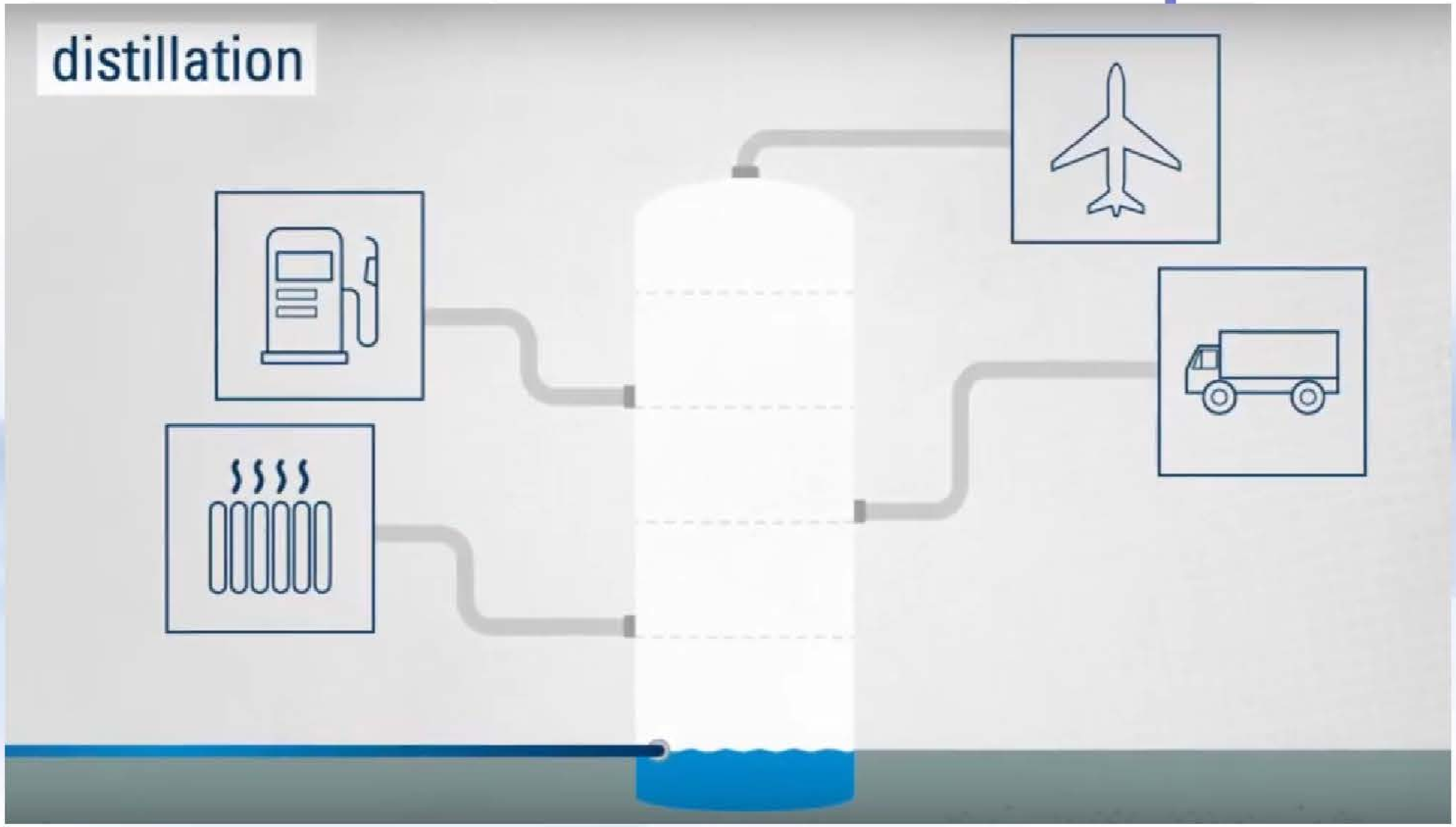
RLC filter assembled on a breadboard



A graphical representation of the model:

- Wires and component geometry not present in the abstracted representation
- Essential features reproduced by the model: connectivity (topology), type of elements, main parameters, input and output ports, variables (input and output voltage signals) and parameters labeled on the diagram

Example:
Crude oil distillation process



- https://www.youtube.com/watch?v=ttKSbXfysKI
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A. The common part, the homomorphism or the analogy between the process and model

B. The homomorphism between the different relations (== theories) mapping the process into different models.

The mapping of the process into a model does not only depend on the chosen theory, but also on the conditions under which the process is being viewed.

The mapped characteristics vary not only with the applied theory but also with the conditions.

Distillation is the most popular and important separation method in the petroleum industries
for purification of final products.
Distillation columns are made up of several components, each of which is used either to transfer heat energy or to enhance mass transfer.

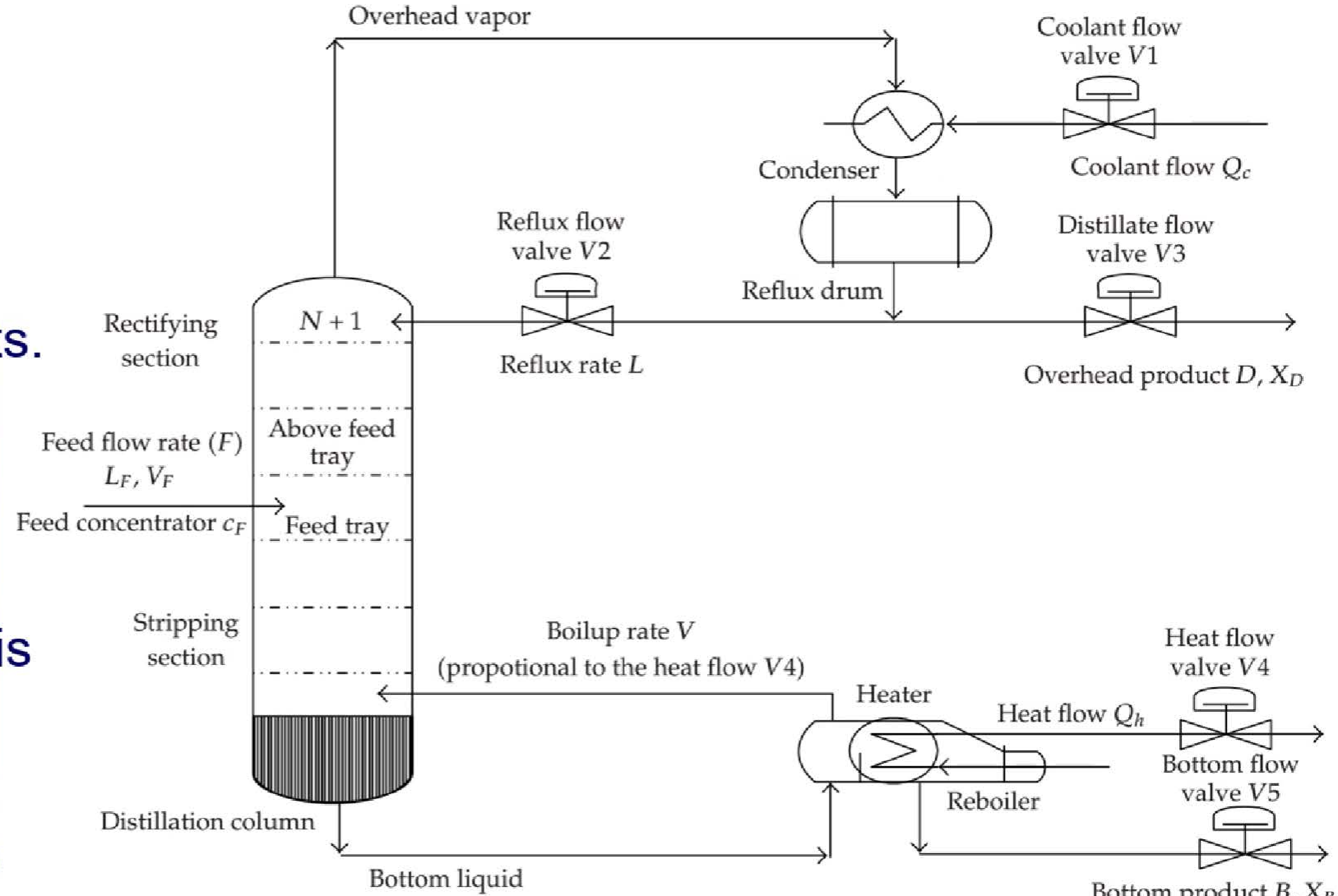


Figure 1: Distillation flowsheet.

Where the system being modelled is more complex, we cannot simply jump from an assumption to an equation.

We must be much more methodical, both when describing the system and when stating assumptions.

Flow diagrams are a visual aid to this end. In their most basic form, they consist of **a series of boxes linked by a network of arrows**.

The boxes represent physical entities which are present in the system, whilst the arrows represent the way these entities inter-relate.

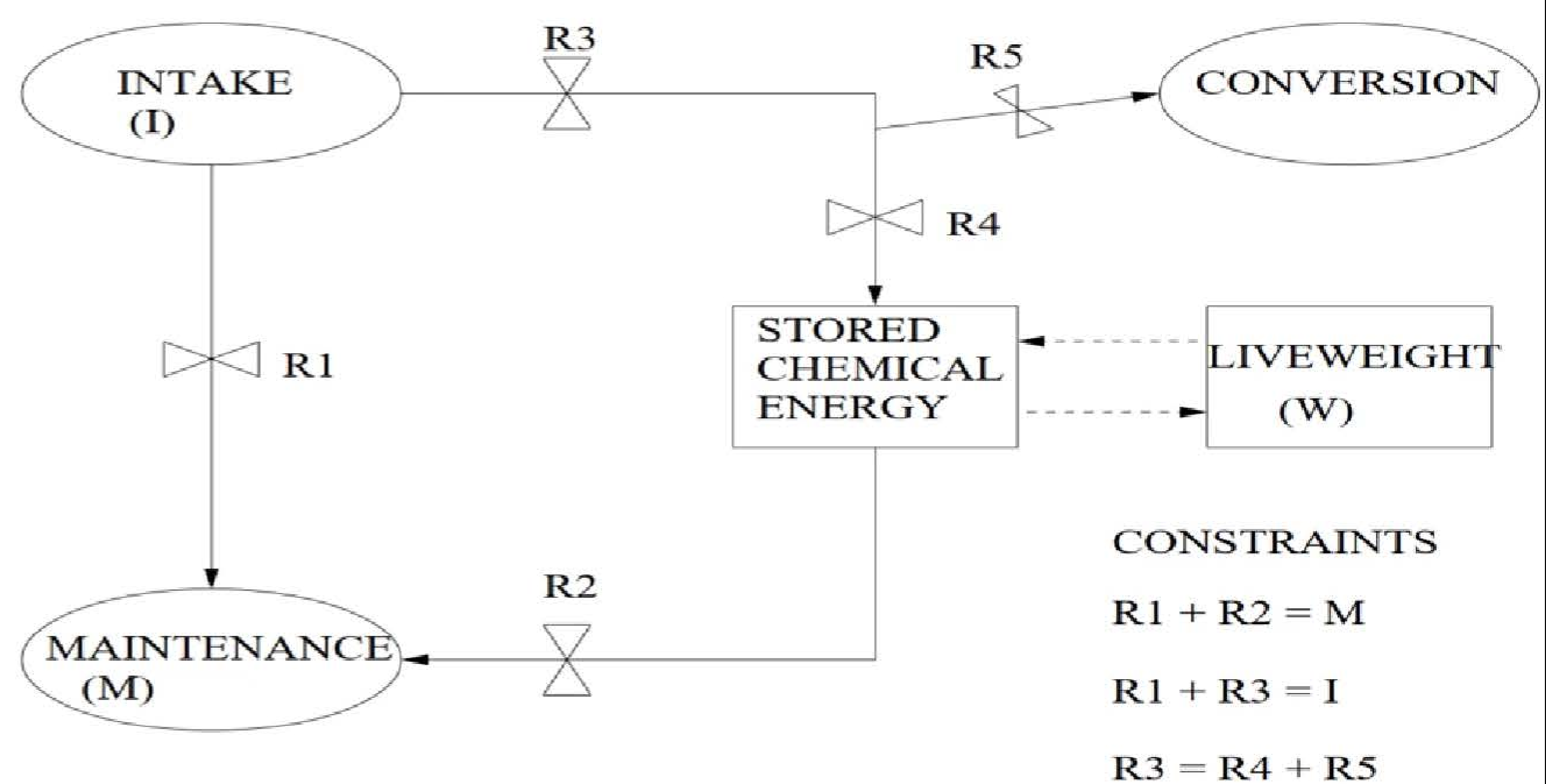
□ state or level variables

○ source or sink

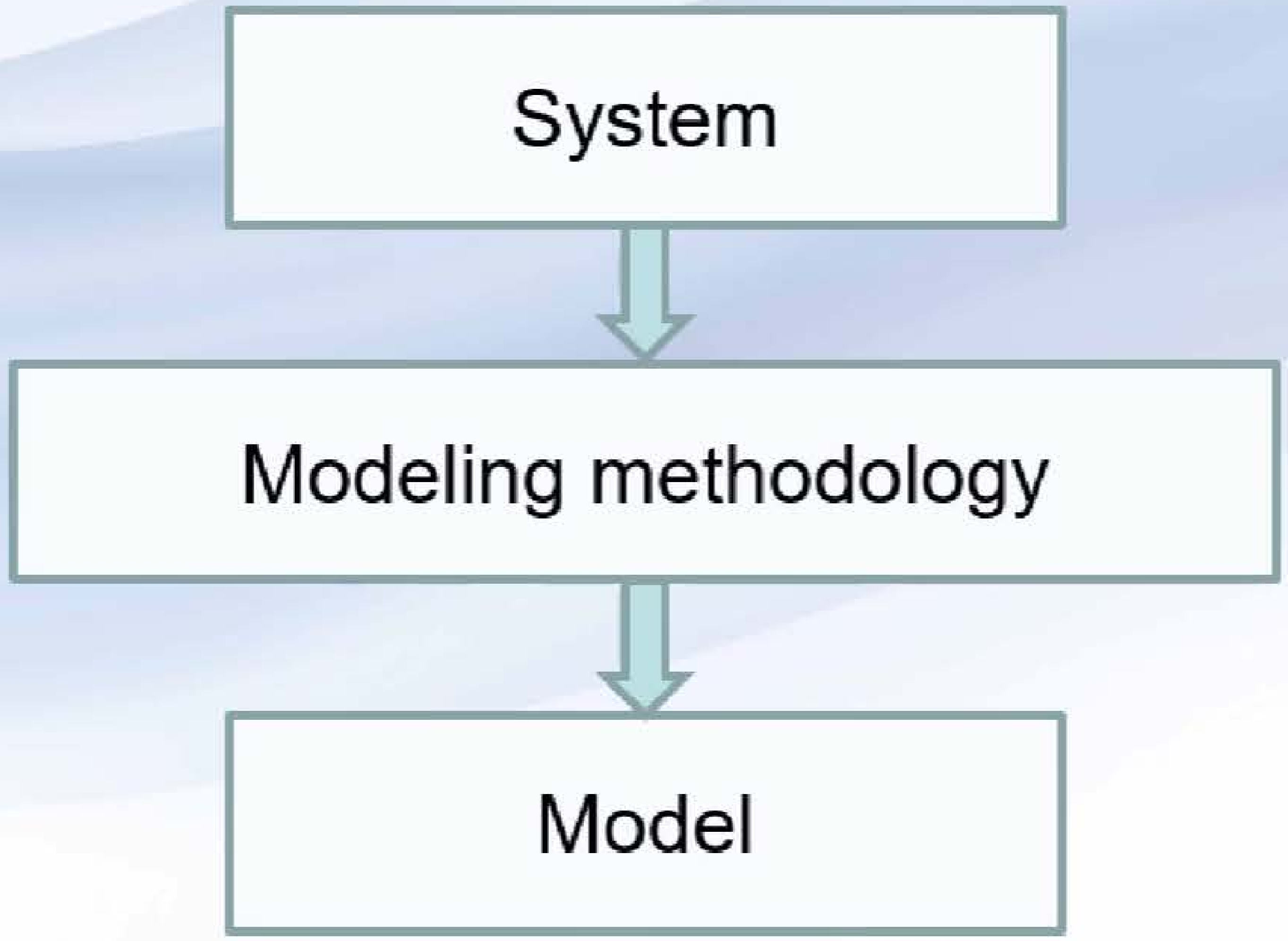
→ channel of material flow

- - → channel of information flow

⋈ control on rate of flow



- Modeling methodology: Transforming a system into a model



- What do we mean by the term *model?*
- *In essence, it is a representation* of reality involving some degree of approximation.
- Models can take many ***forms***:

- conceptual
- mental
- verbal
- physical
- statistical
- mathematical
- logical
- graphical

A **process flow diagram (PFD)** is a diagram commonly used in chemical and process engineering to indicate the general flow of plant processes and equipment. The PFD displays the relationship between *major* equipment of a plant facility and does not show minor details such as piping details and designations. Another commonly used term for a PFD is a ***flowsheet***.

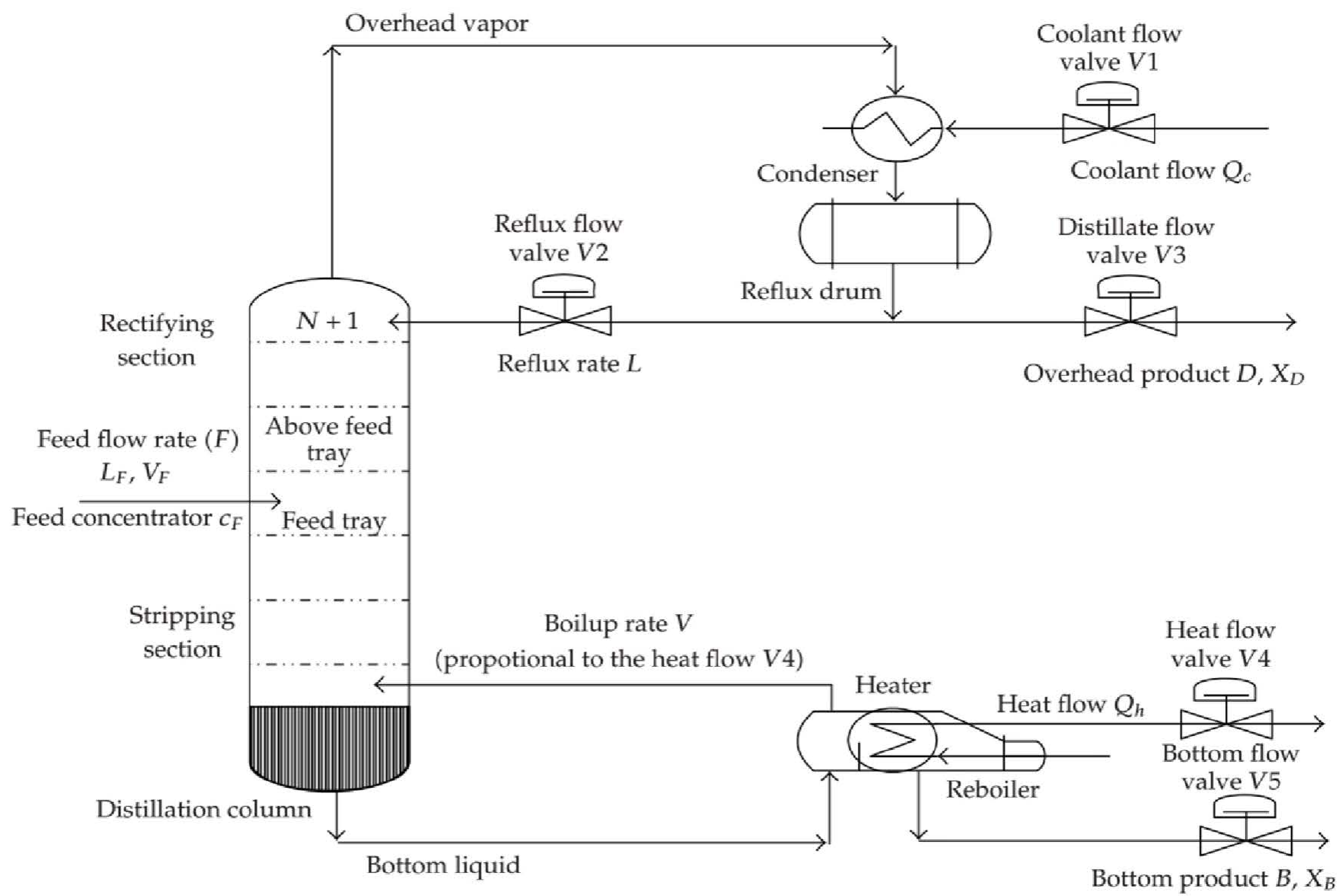
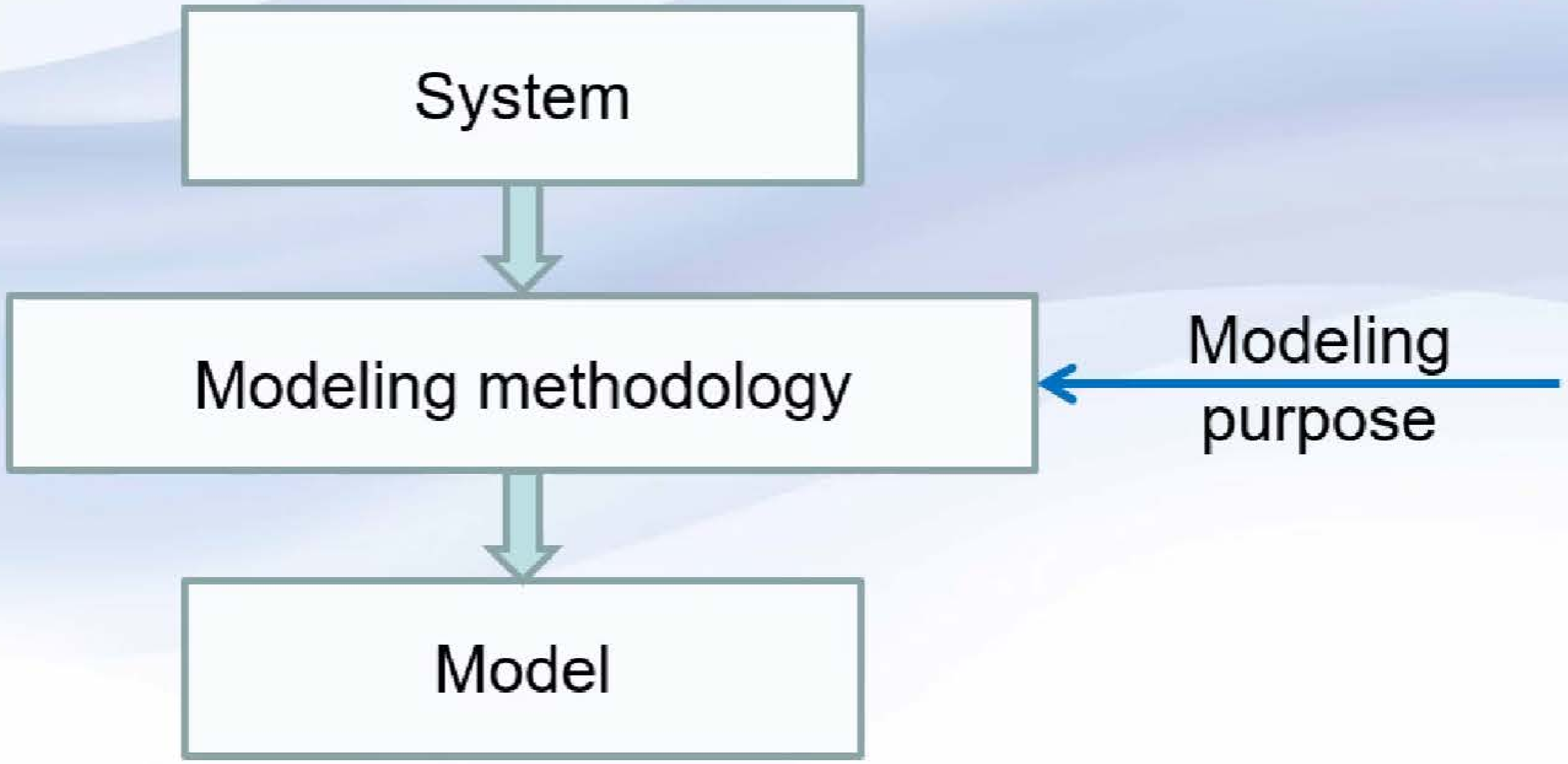


Figure 1: Distillation flowsheet.

- The purpose of modeling: <u>A key driver</u> of modeling methodology



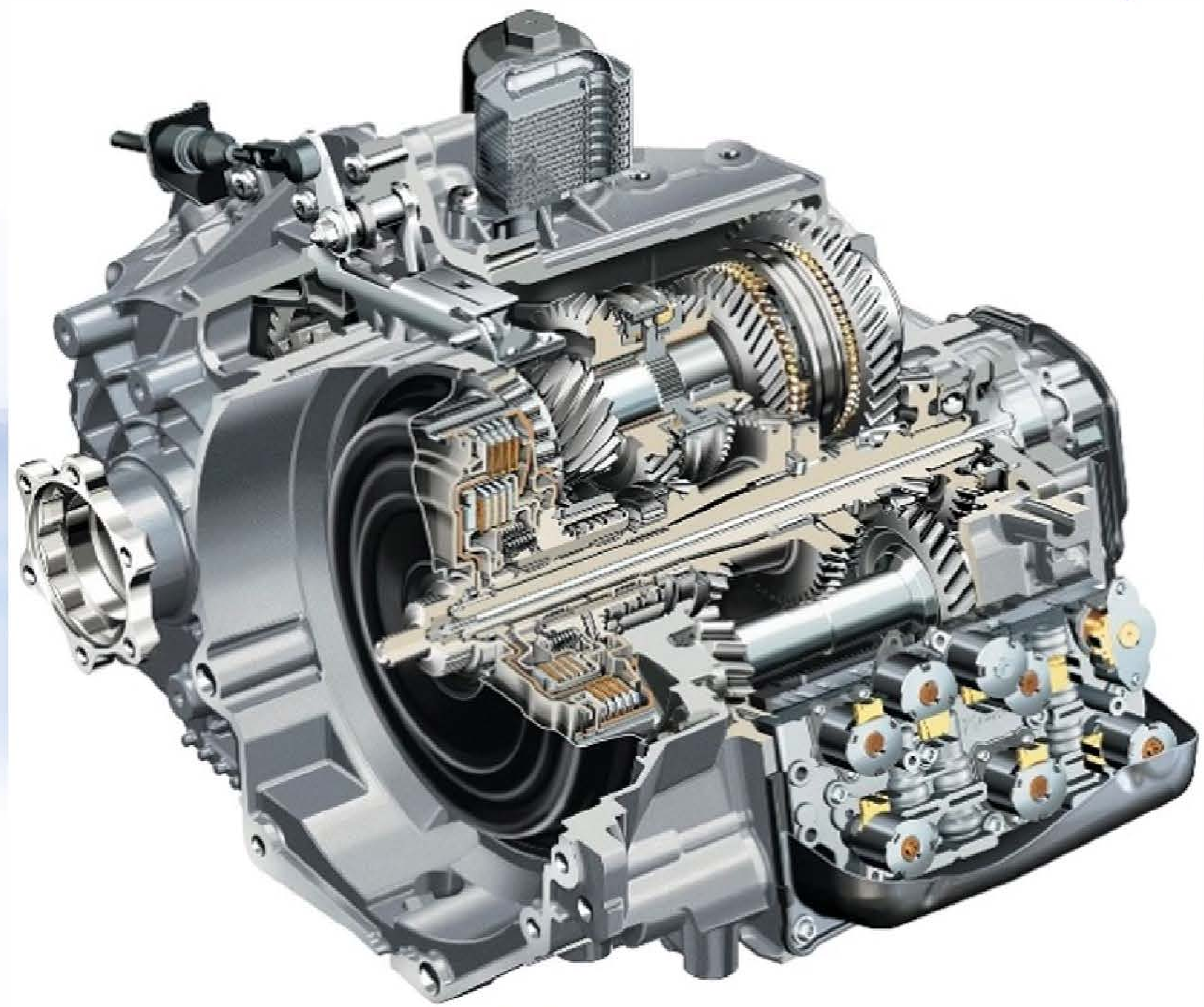
General purpose of a model:

- to describe
- to interpret
- to predict
- to explain.

More specific purposes:

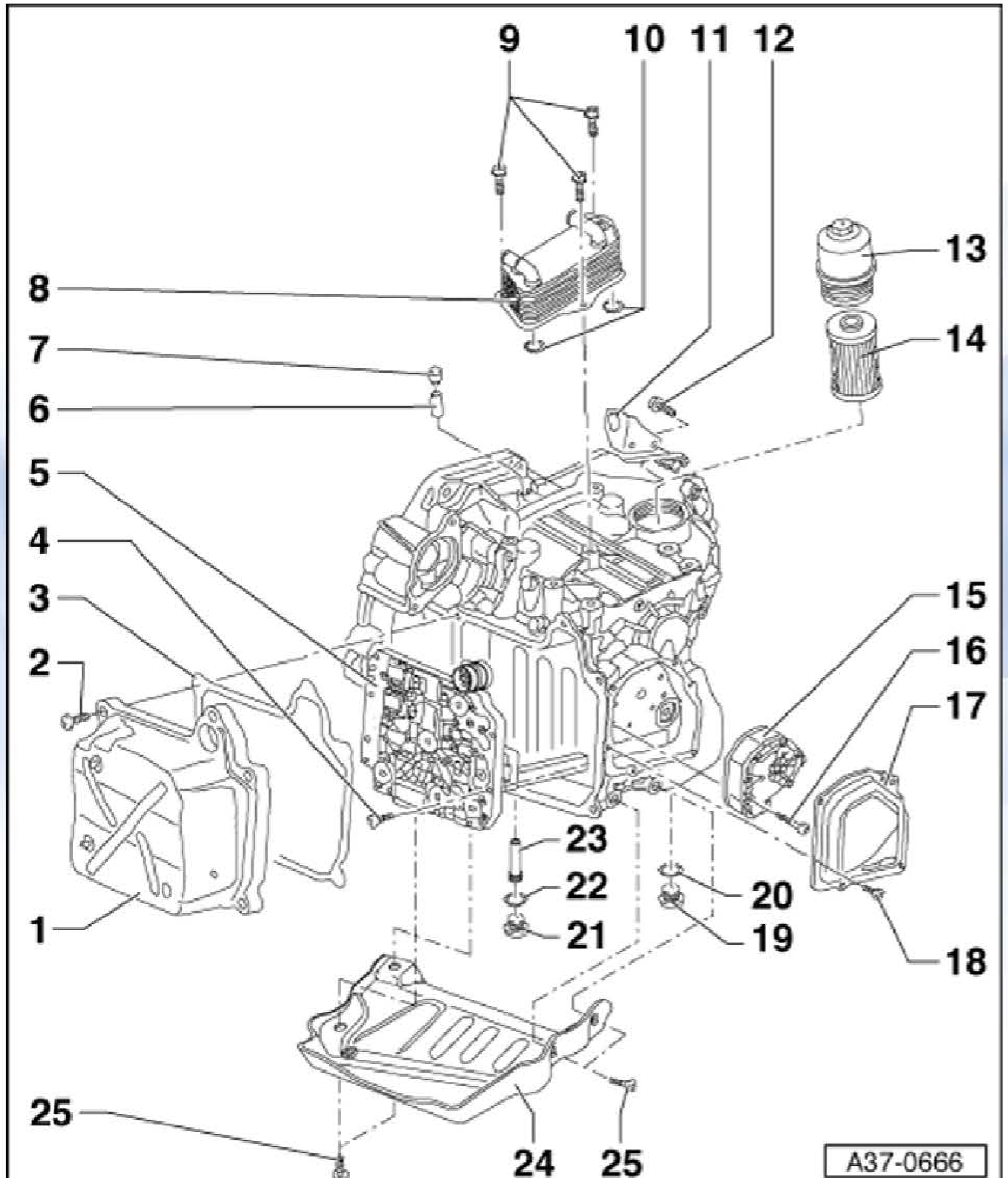
- aiding understanding
- testing hypotheses
- measuring inferences
- teaching
- simulating
- examining experimental design

Example: Gearbox system representation for different purposes



Section through the **REAL SYSTEM**: DOBLE CLUTCH GEARBOX

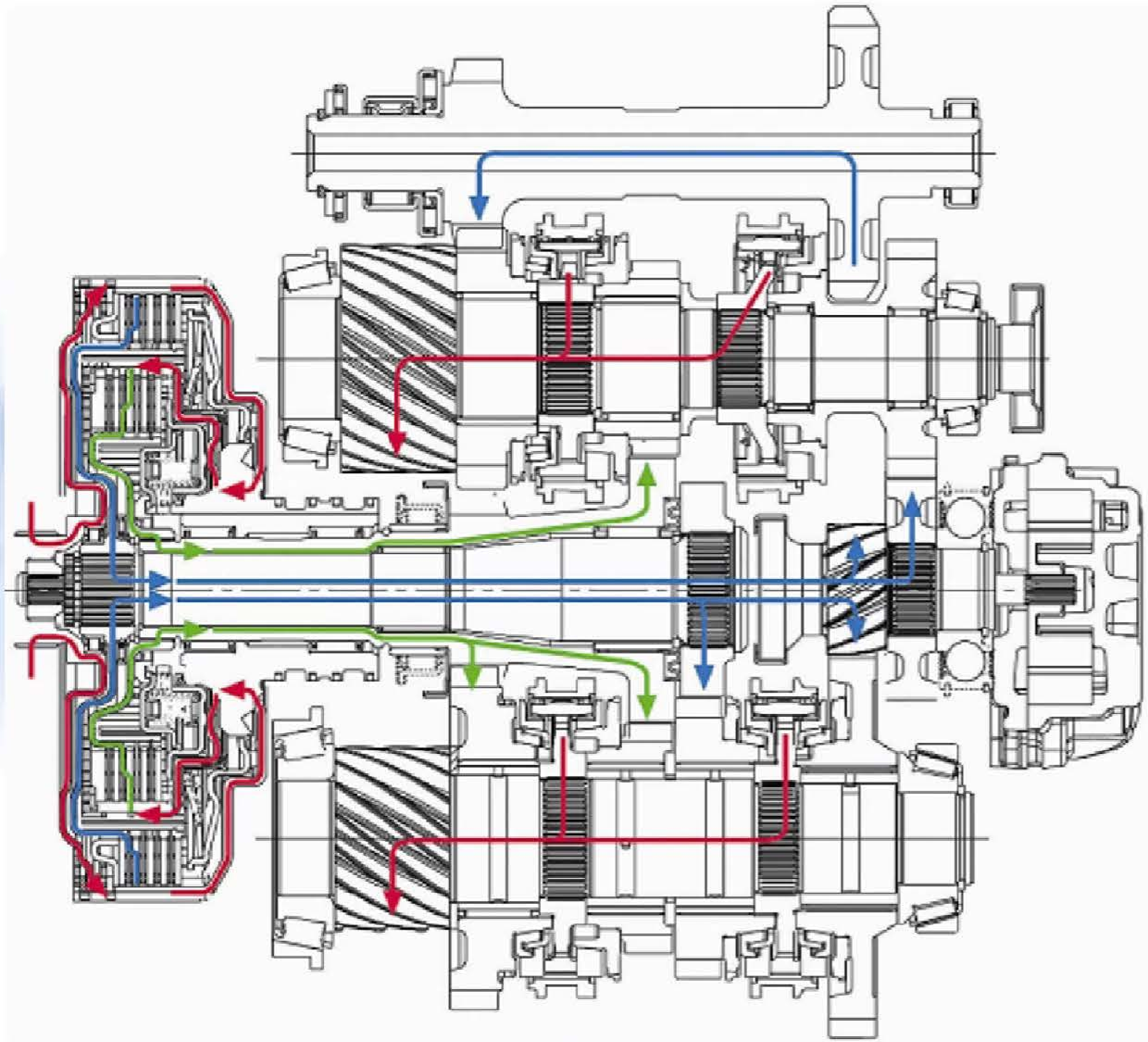
Example: Gearbox system representation for different purposes



1 - Oil pan
2 - Bolt
3 - Gasket
q Renew
4 - Bolt
5 - Mechatronic unit for dual clutch gearbox
6 - Breather pipe
7 - Breather cap
15 - Gear oil pump
16 - Bolt
17 - Cover for gear oil pump
18 - Bolt
24 - Guard plate
25 - Bolt

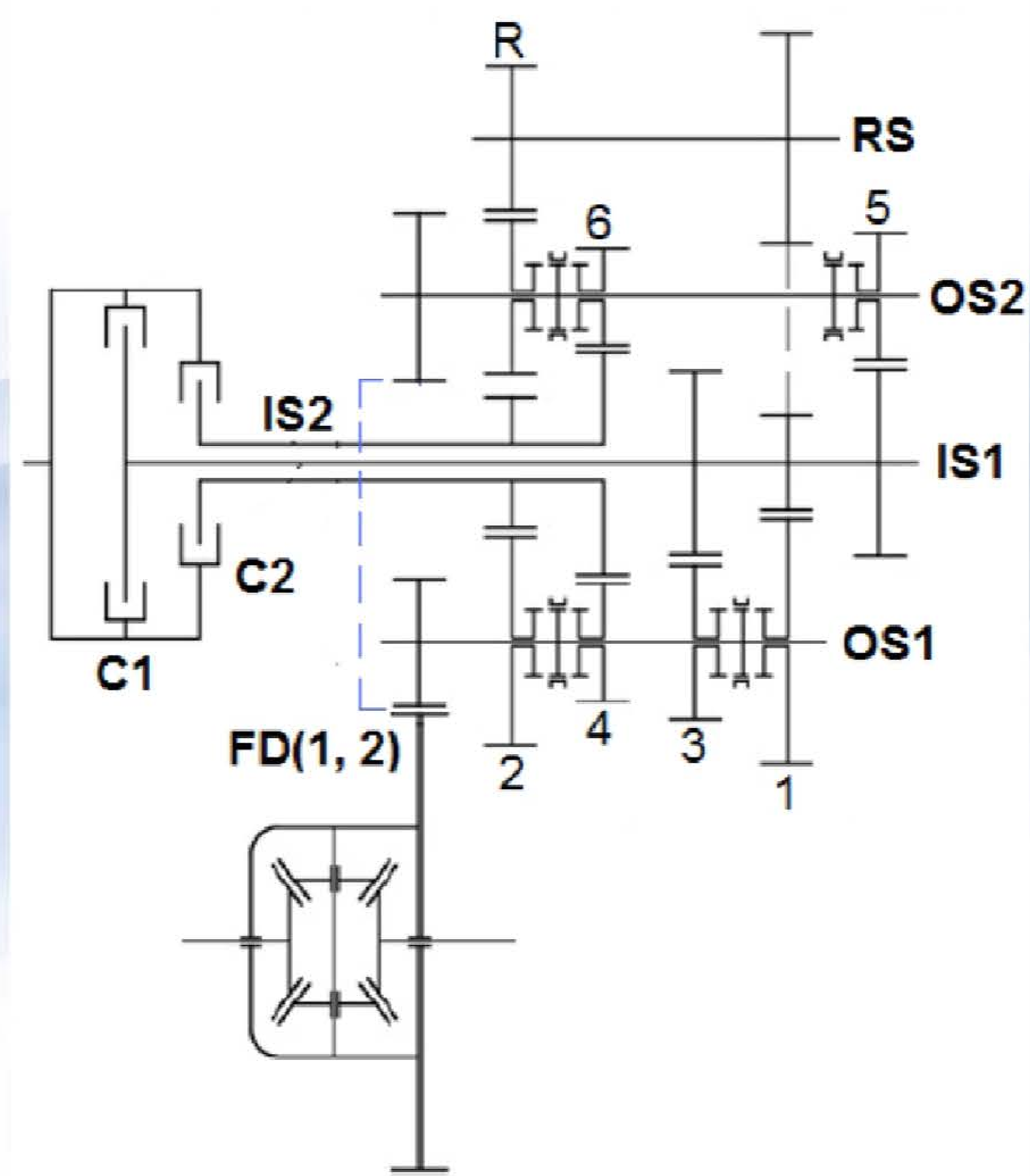
Exploded view **REPRESENTATION** for <u>servicing and maintenance purposes</u>

Example: Gearbox system representation for different purposes



Cross section **REPRESENTATION** for teaching and analysis purposes

Example: Gearbox system representation for different purposes



Layout **REPRESENTATION** as <u>stick diagram</u> - schematic representation

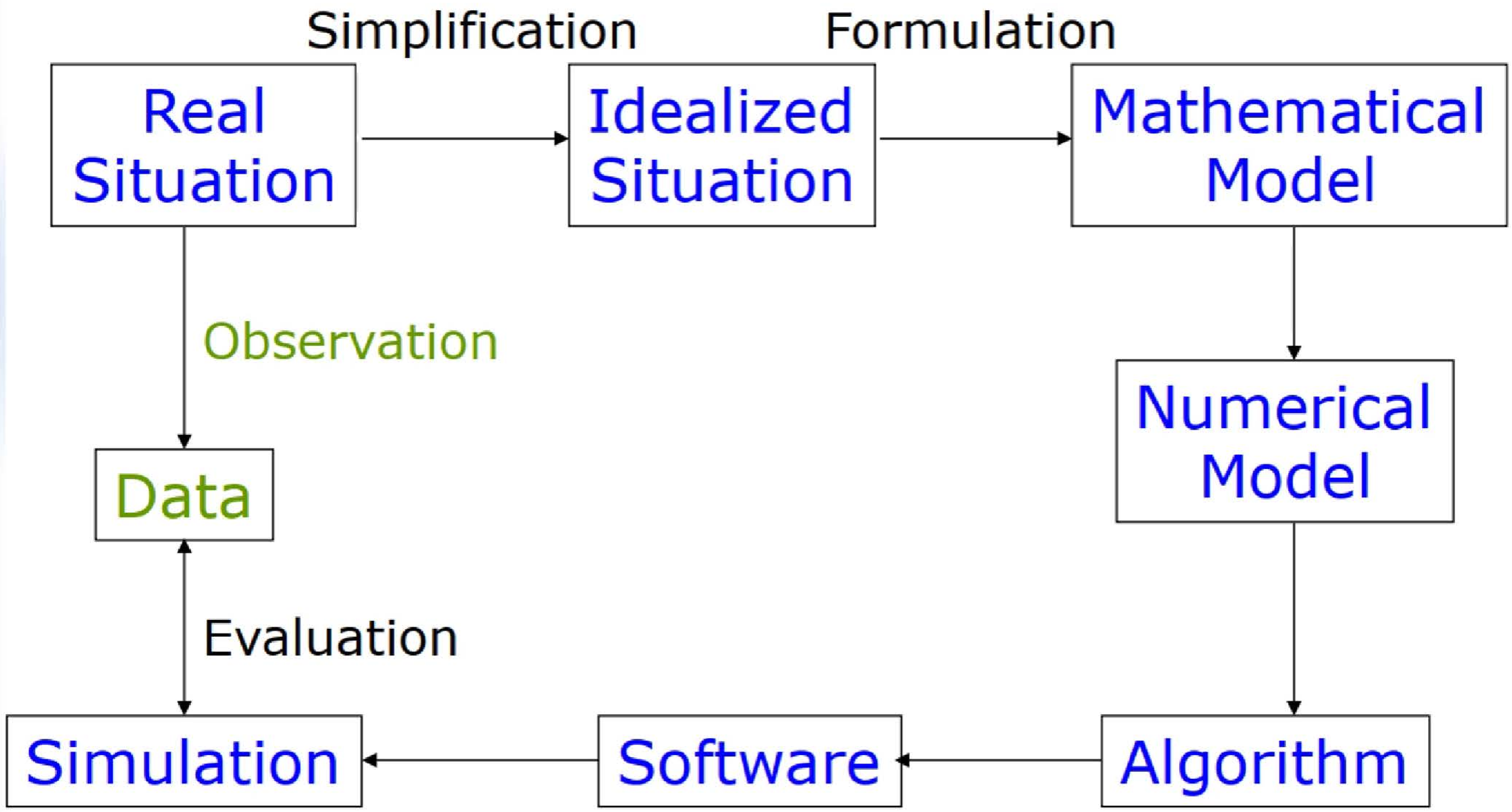
Use of mathematical models

- Answering questions that need **quantitative answers**
- Design of engineering components and systems
- Analysis of events that **have not yet occurred**
- **Exploring inaccessible parts** of bodies
- Minimizing **risks**

Developing a mathematical model

1. **Specify the purpose of the model:**
   define the problem;
   decide which aspects of the problem to investigate.
2. **Create the model:**
   state assumptions;
   choose variables and parameters;
   formulate mathematical relationships.
3. **Do the mathematics:**
   solve equations;
   draw graphs;
   derive results.
4. **Interpret the results:**
   collect relevant data;
   describe the mathematical solution in words;
   decide what results to compare with reality.
5. **Evaluate the model:**
   test the model by comparing its predictions with reality;
   criticise the model.

Developing a mathematical model and using it for simulation



Approaches to developing a **mathematical model**

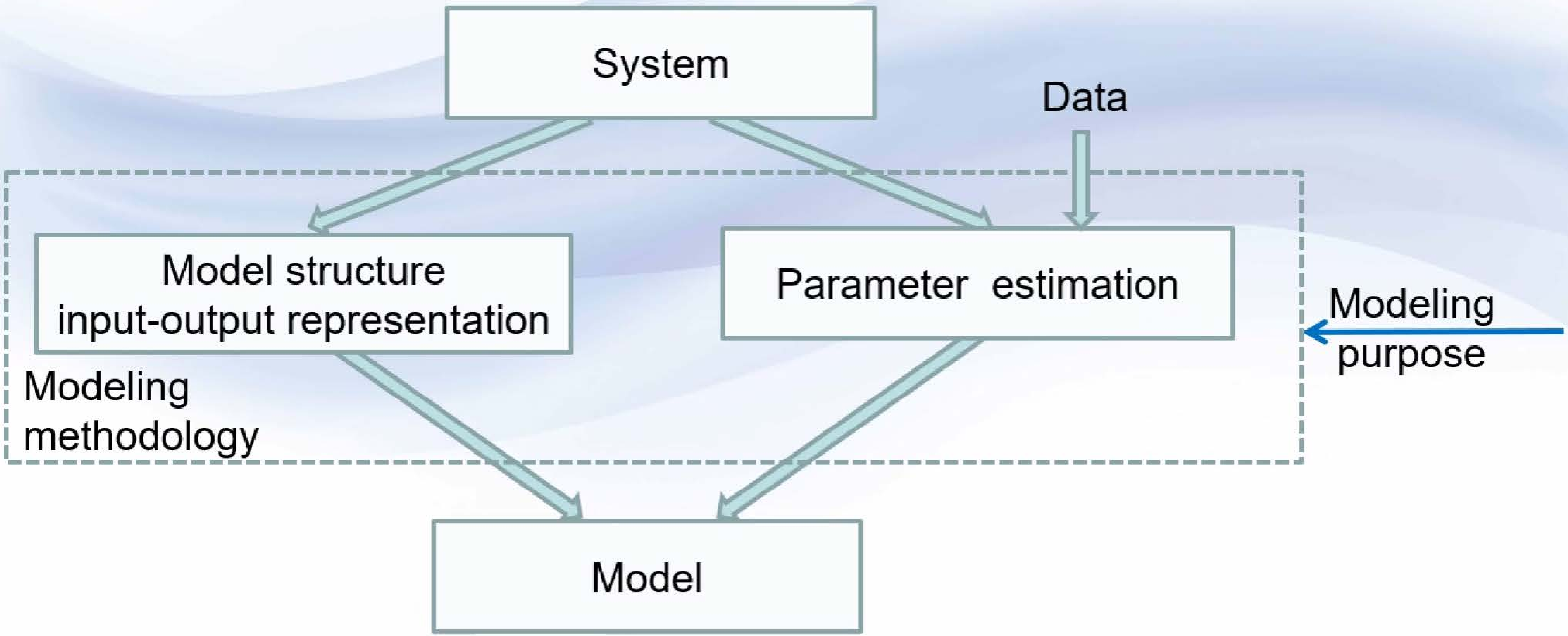
- The first is based on experimental data and is essentially a ***data driven*** approach.
- The second is based on a fundamental understanding of the physical and chemical processes that give rise to the resultant experimental data. It is referred to as ***modelling the system***.

MODELLING THE DATA

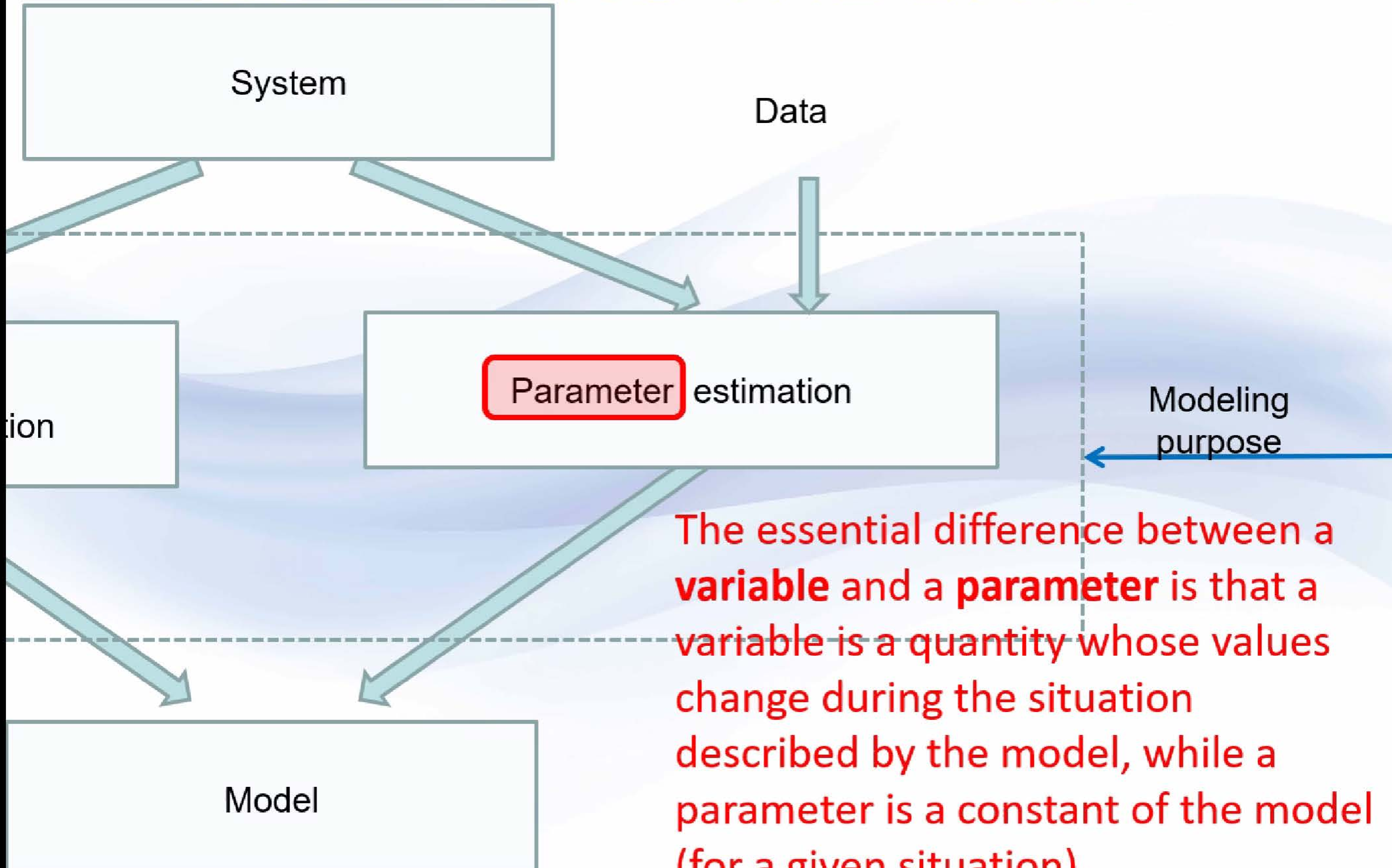
- Models that are based on experimental data are generally known as ***data-driven*** or ***black box models***.
- These models look for ***quantitative descriptions*** of the systems based on input-output (I/O) descriptions ***derived from experimental data collected on the system/process***.
- These are ***mathematical descriptions of data***, with only implicit correspondence to the underlying processes.

MODELLING THE DATA

- A methodological framework



MODELLING THE DATA

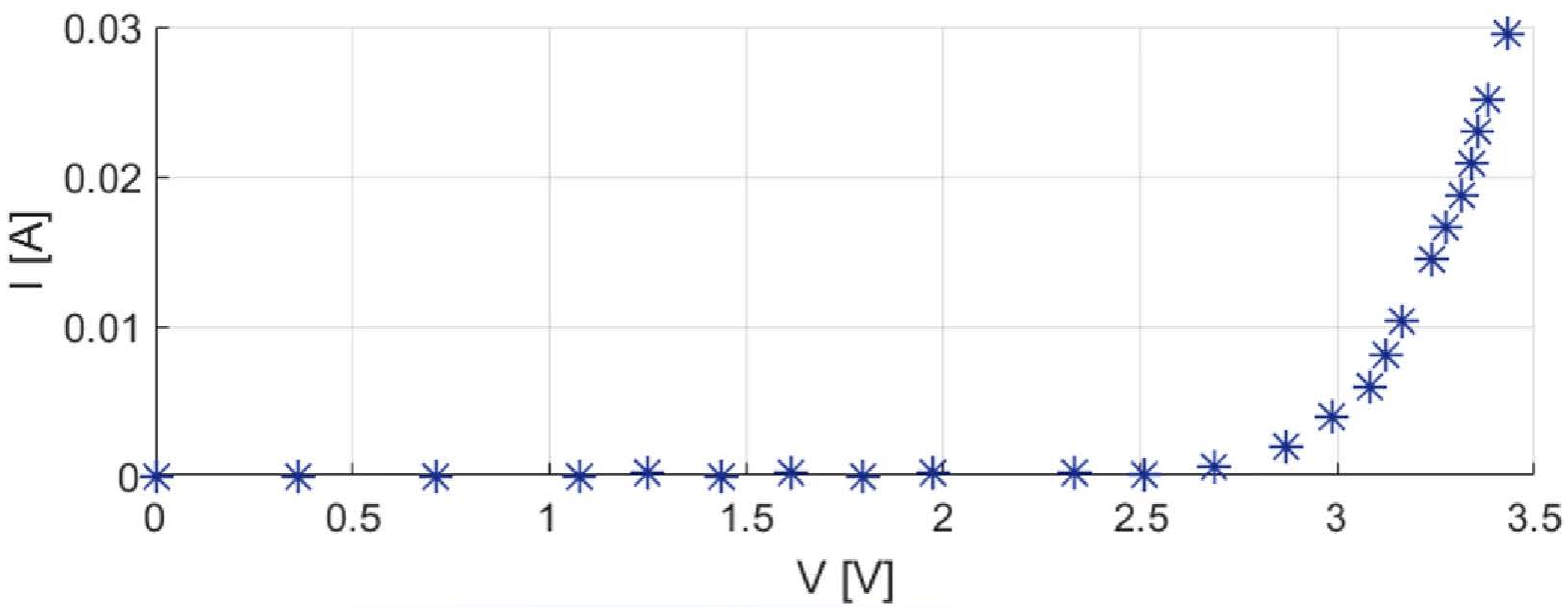


The essential difference between a **variable** and a **parameter** is that a variable is a quantity whose values change during the situation described by the model, while a parameter is a constant of the model (for a given situation).

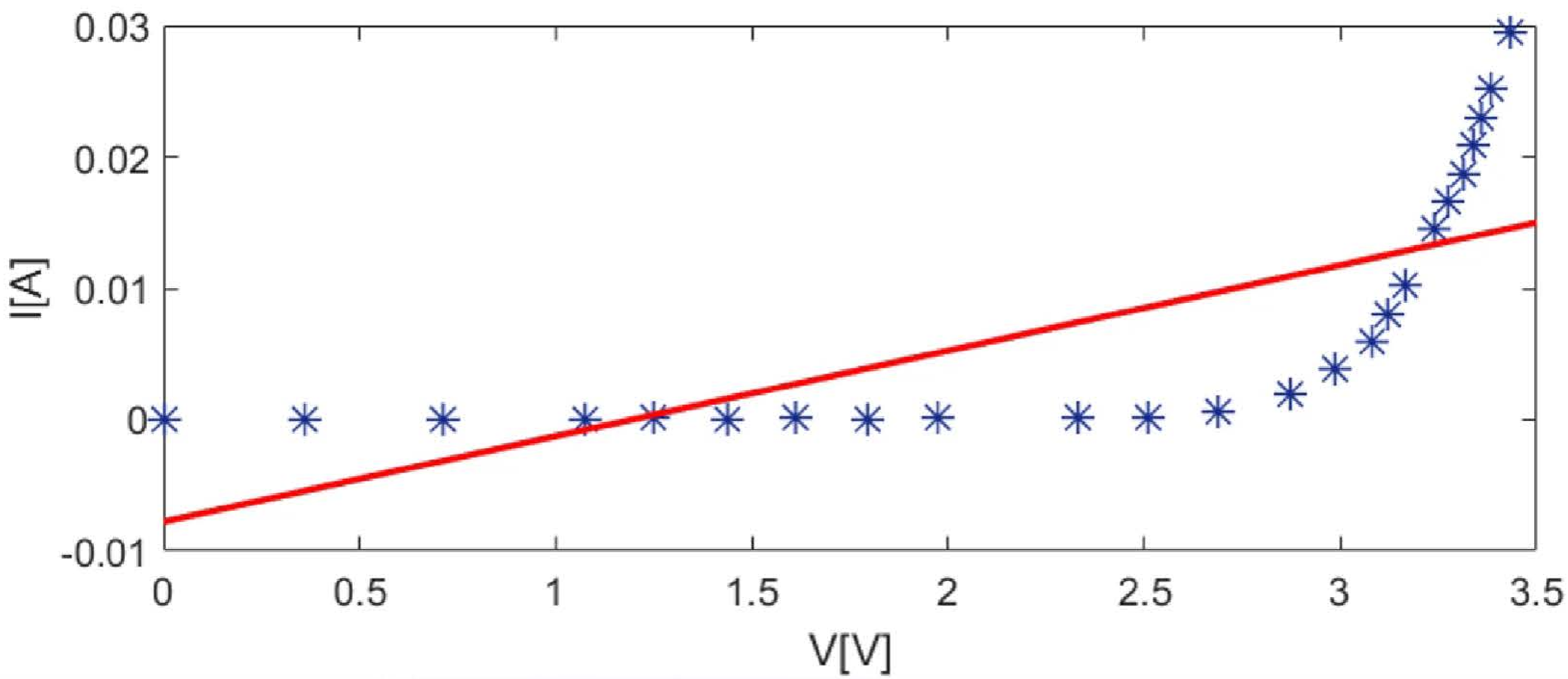
Why should we use data models?

- they are particularly appropriate where there is a lack of knowledge of the underlying processes,
- whether ***a priori* knowledge or knowledge are acquired *directly through measurement*.**
- Sometimes just an *overall I/O representation of the system's dynamics is needed*, without knowing specifically how the internal process mechanisms gave rise to such I/O behavior.

Example: LED forward bias characteristics

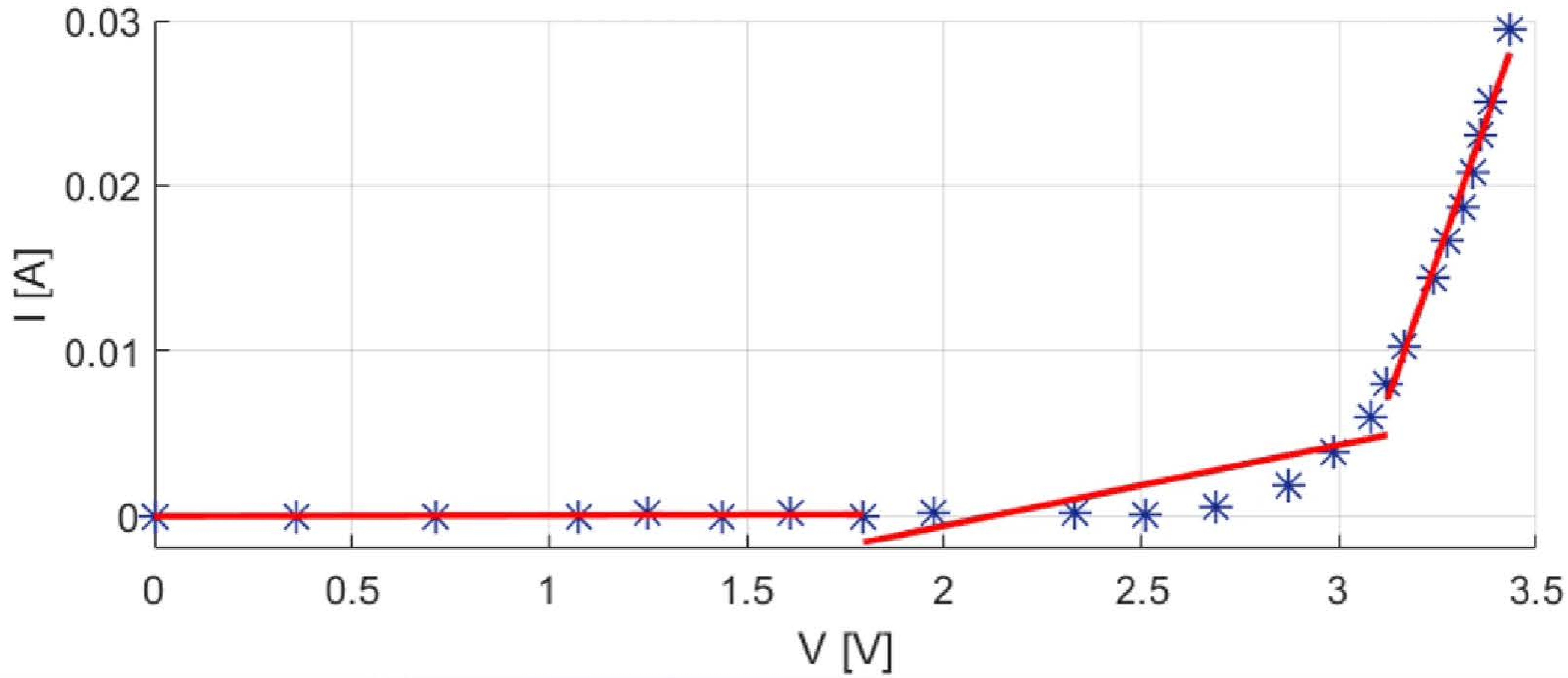


Linear approximation



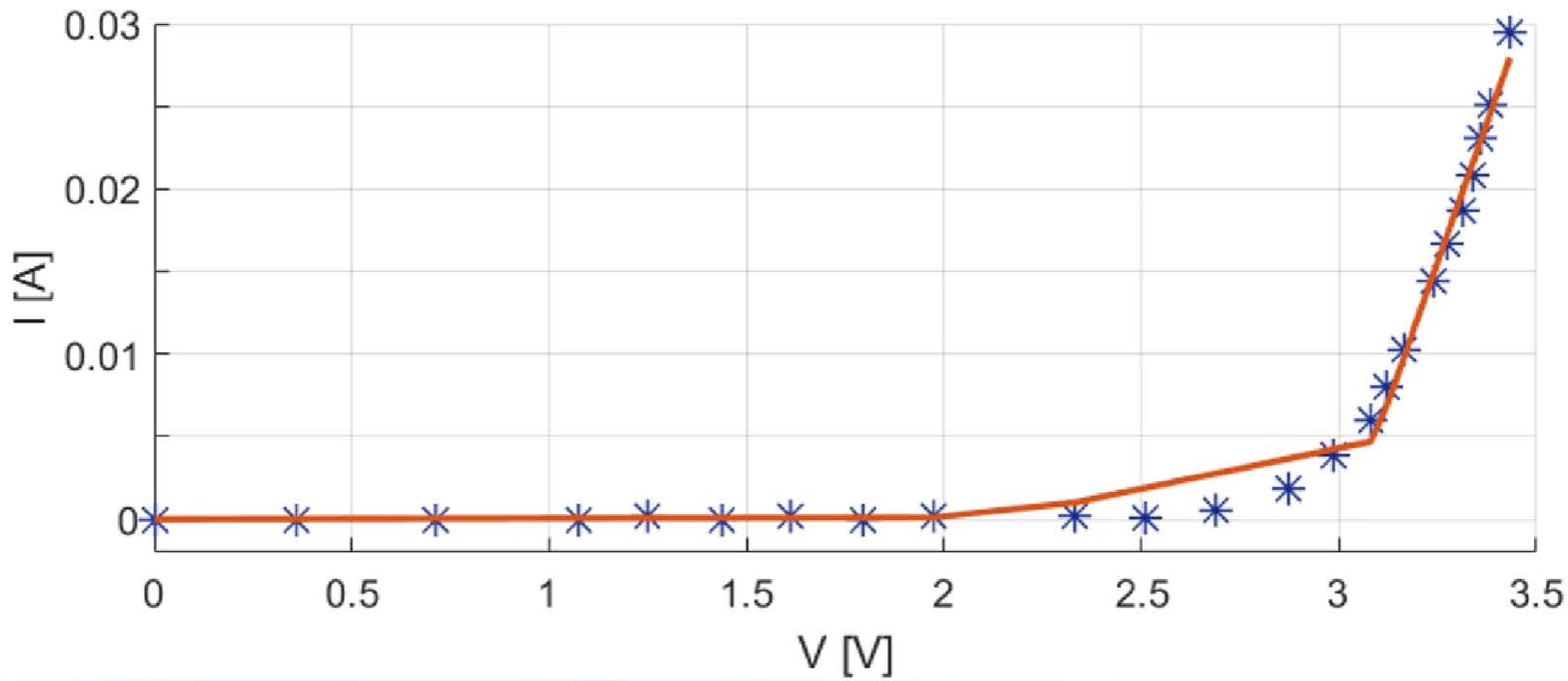
$$I_f = 0.0065V - 0.0078$$

Piecewise linear model



$$I_f = \begin{cases} 0.5832 \cdot 10^{-4} V - 0.1009 \cdot 10^{-4}, & V \in [0, 1.80] \\ 0.0049\, V - 0.0104, & V \in (\,1.80, 3.16] \\ 0.0675\, V - 0.2038, & V \in (3.16, 3.43] \end{cases}$$

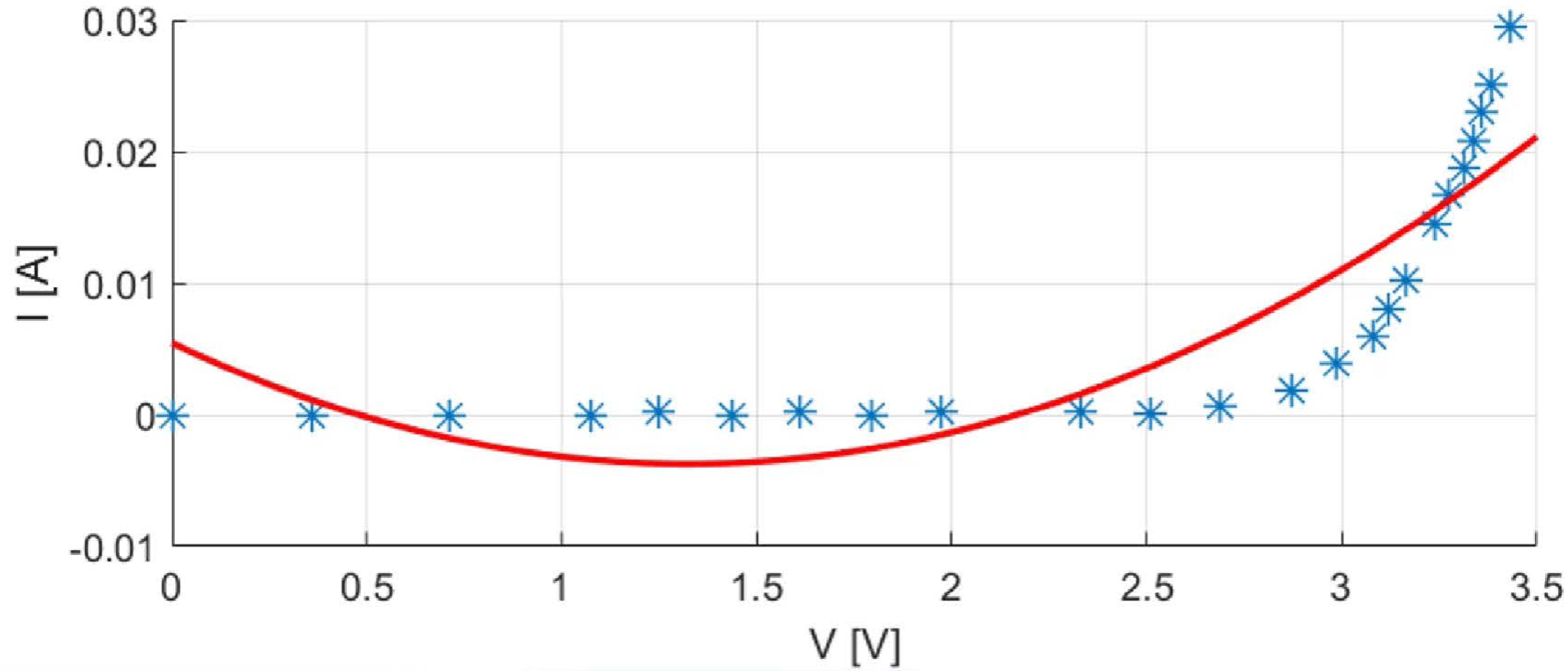
Characteristic curve approximated as a broken line (continuous piecewise linear model)



$$I_f = \begin{cases} 0.5832 \cdot 10^{-4} V - 0.1009 \cdot 10^{-4}, & V \in [0, 2.15] \\ 0.0049\, V - 0.0104, & V \in (2.15, 3.09] \\ 0.0675\, V - 0.2038, & V \in (3.09, 3.43] \end{cases}$$

Quadratic approximation

If the class of quadratic polynomials is considered, then a new *structure of the model* is imposed and this time the three coefficients act as *model parameters*



$$I_f = 0.005248 \cdot V^2 - 0.01389 \cdot V + 0.005448$$

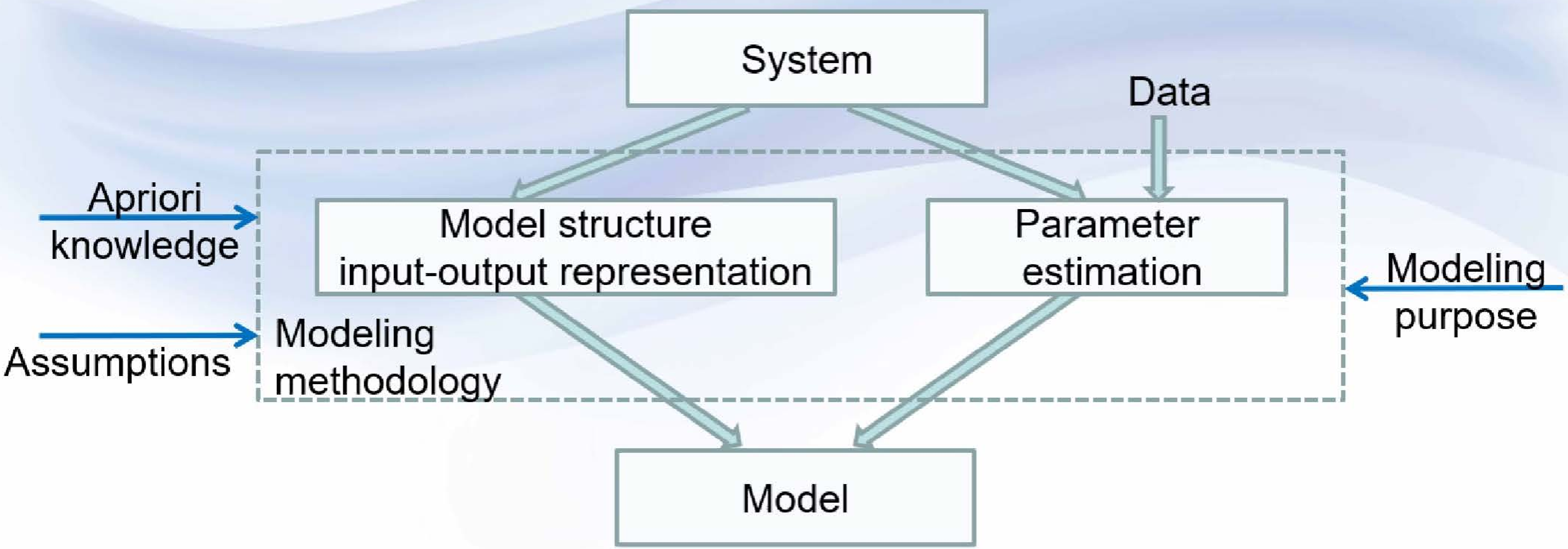
MODELLING THE SYSTEM

– when modeling the system there is an attempt to explicitly represent the underlying processes, albeit at an appropriate level of approximation and resolution.

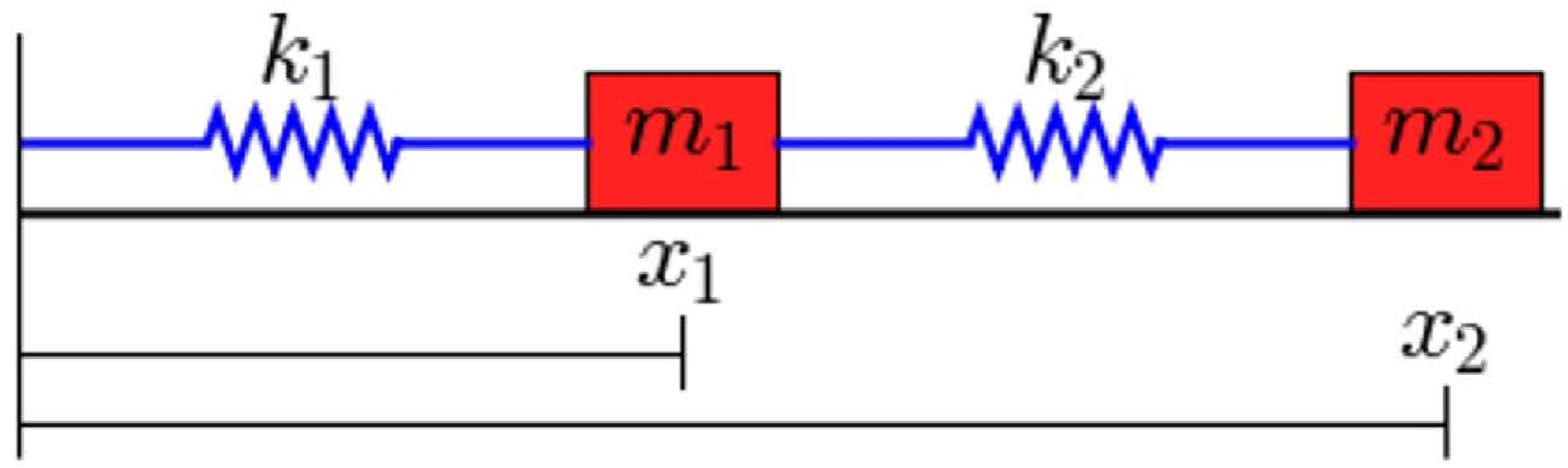
– The degree of approximation will be largely determined by the availability of *a priori knowledge and the nature of the* assumptions that can be made.

MODELLING THE SYSTEM

- Modeling the system: A methodological framework



Example: double spring system



VARIABLES

- x_1, x_2 = position (left edge) of blocks
- v_1, v_2 = velocity of blocks
- F_1, F_2 = force experienced by blocks
- L_1, L_2 = how much spring is stretched

PARAMETERS

- m_1, m_2 = mass of blocks
- w_1, w_2 = width of blocks
- k_1, k_2 = spring constants
- R_1, R_2 = rest length of springs

MATHEMATICAL MODEL in the form of second order differential equations

$$m_1 x_1'' = -k_1 (x_1 - R_1) + k_2 (x_2 - x_1 - w_1 - R_2)$$
$$m_2 x_2'' = -k_2 (x_2 - x_1 - w_1 - R_2)$$

https://www.myphysicslab.com/springs/double-spring-en.html

MODELLING THE SYSTEM

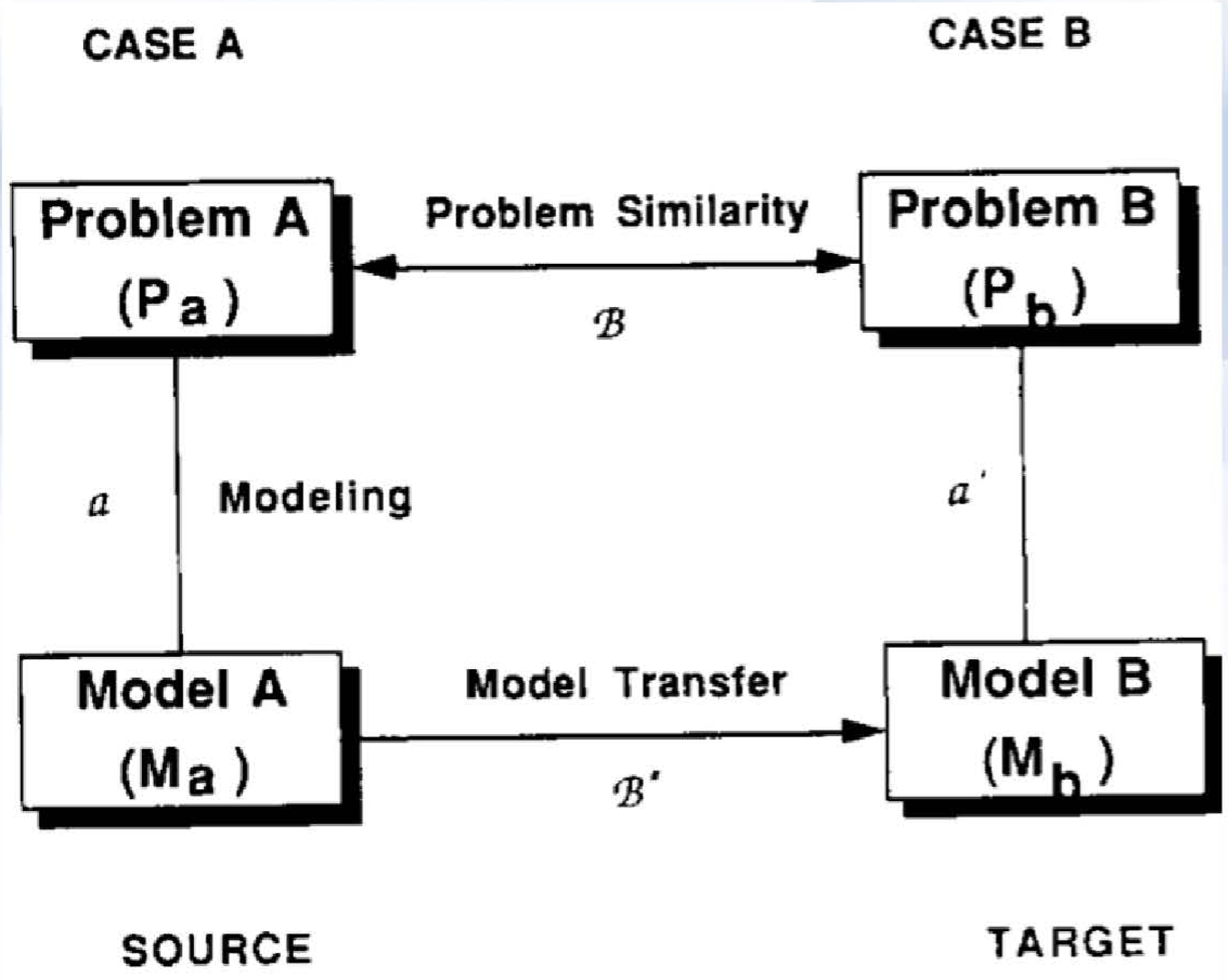
Models of the system, that is, models that are ***process based***, may be categorized in a number of ways according to the included attributes:

- static v. dynamic models
- deterministic v. stochastic
- time-invariant v. time-varying
- lumped v. distributed
- linear v. nonlinear
- continuous v. discrete models.

MODELLING BY ANALOGY

Modelling by analogy (analogical modelling) is a process by which analogical reasoning is adopted for model construction.

A model is constructed for a problem based on the similarity of the problem to previously solved problems.



A key issue in modeling by analogy is to identify similarity. Similarity is defined in two dimensions: **entity** and **structure** Problems may be similar in **the entities they consist** and / or **the way** those entities **are related**.

SIMULATION

"simulations are closely related to dynamic models. More concretely, a simulation results when the equations of the underlying dynamic model are solved. This model is designed to imitate the time-evolution of a real system.

To put it another way, *a simulation imitates one process by another process*. […]

If the simulation is run on a computer, it is called a *computer simulation*" (Hartmann 1996)

SIMULATION

Simulation is the process of solving the model (i.e., the equations that are the realization of the model) to examine its output behavior.

- It involves examining the time evolution of one or more of the variables; performing computer experiments on the model.

<u>When is simulation required</u>?

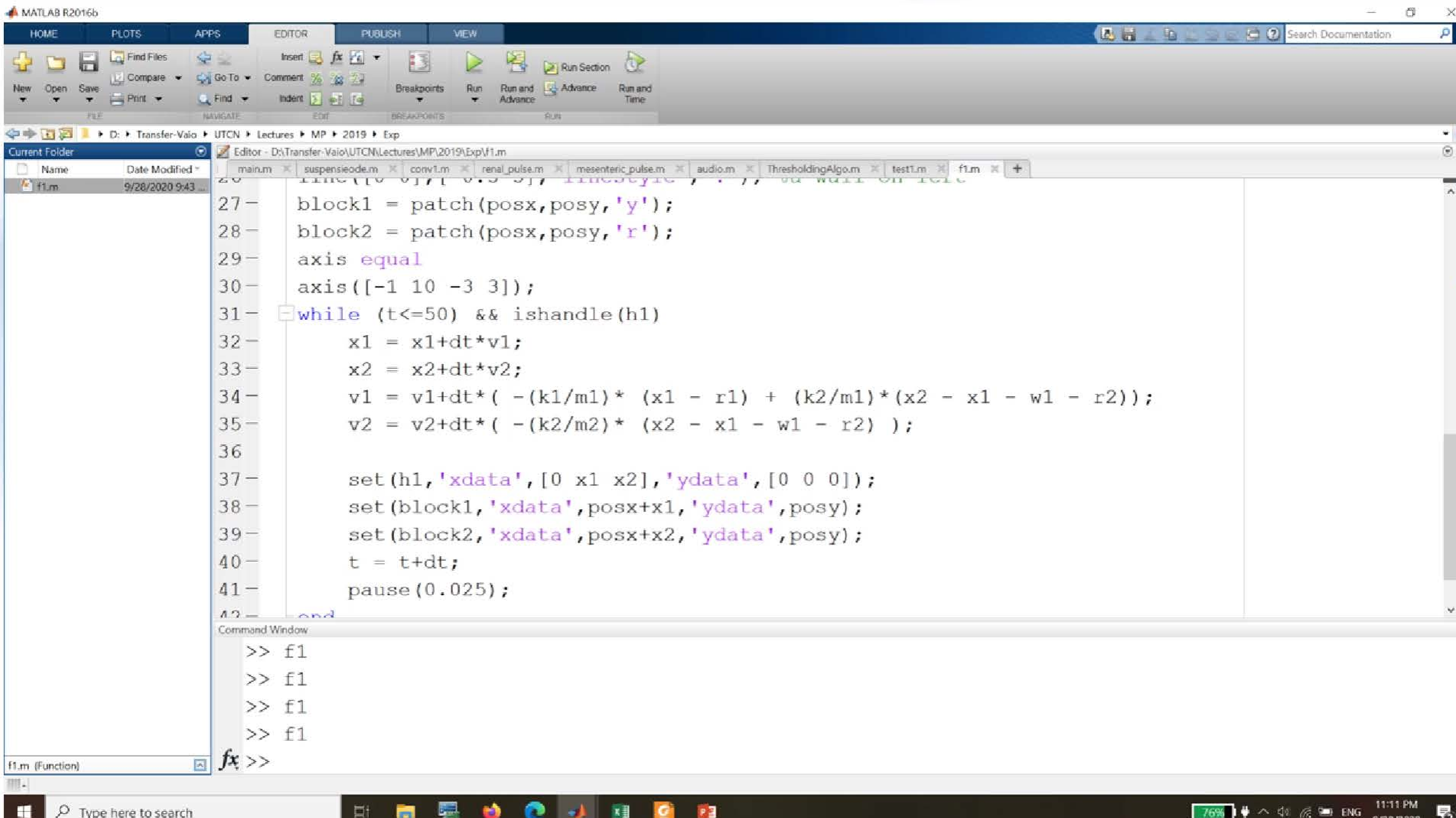
- during the process of model building
- once the model is completed

Example: Matlab simulation of double spring system

Steps:

1) Write **the equations of the model**
2) Use a **numerical method** in order to get an *approximated* solution of the differential equation at **a given time moment,** an then propagate this toward a solution at a new time moment (after a **time step** dt)
3) Apply step 2 in an **iterative manner** for **constructing time series of the position variables**
4) Create a sequence of graphical representations
5) Display the sequence of representations as a movie

Example: Matlab simulation of double spring system

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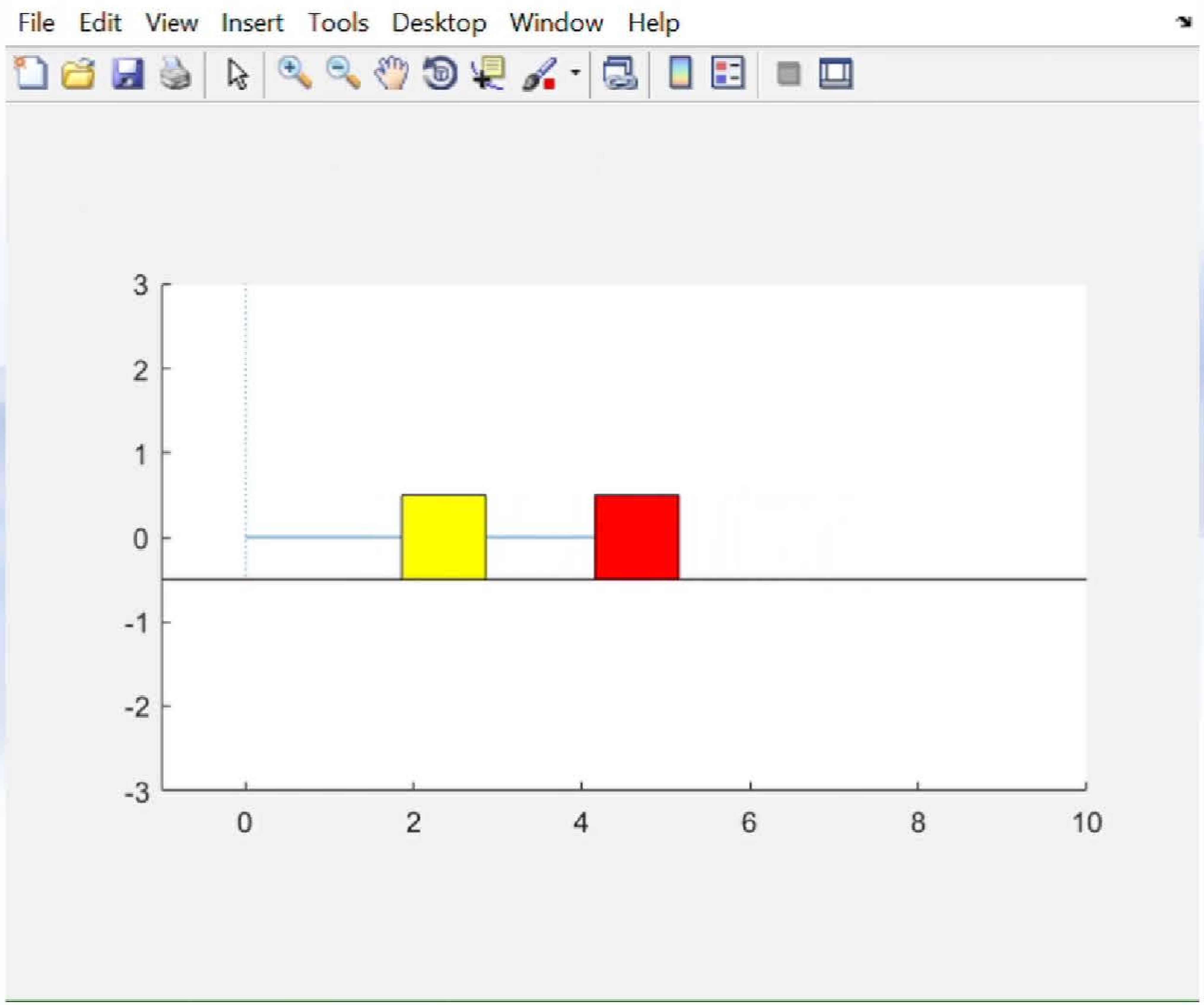
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SIMULATION

During model building, simulation can be performed in order to:

- clarify aspects of system behaviour
- determine whether a proposed model representation is appropriate. This is done by ***comparison of the model response with experimental data*** from the same situation

SIMULATION

When carried out on a **complete, validated model**, simulation yields ***output responses that provide information on system behavior***.

Depending on the modeling purpose, this information assists in:

- describing the system
- predicting behavior
- yielding additional insights (i.e., explanations).

MODEL IDENTIFICATION

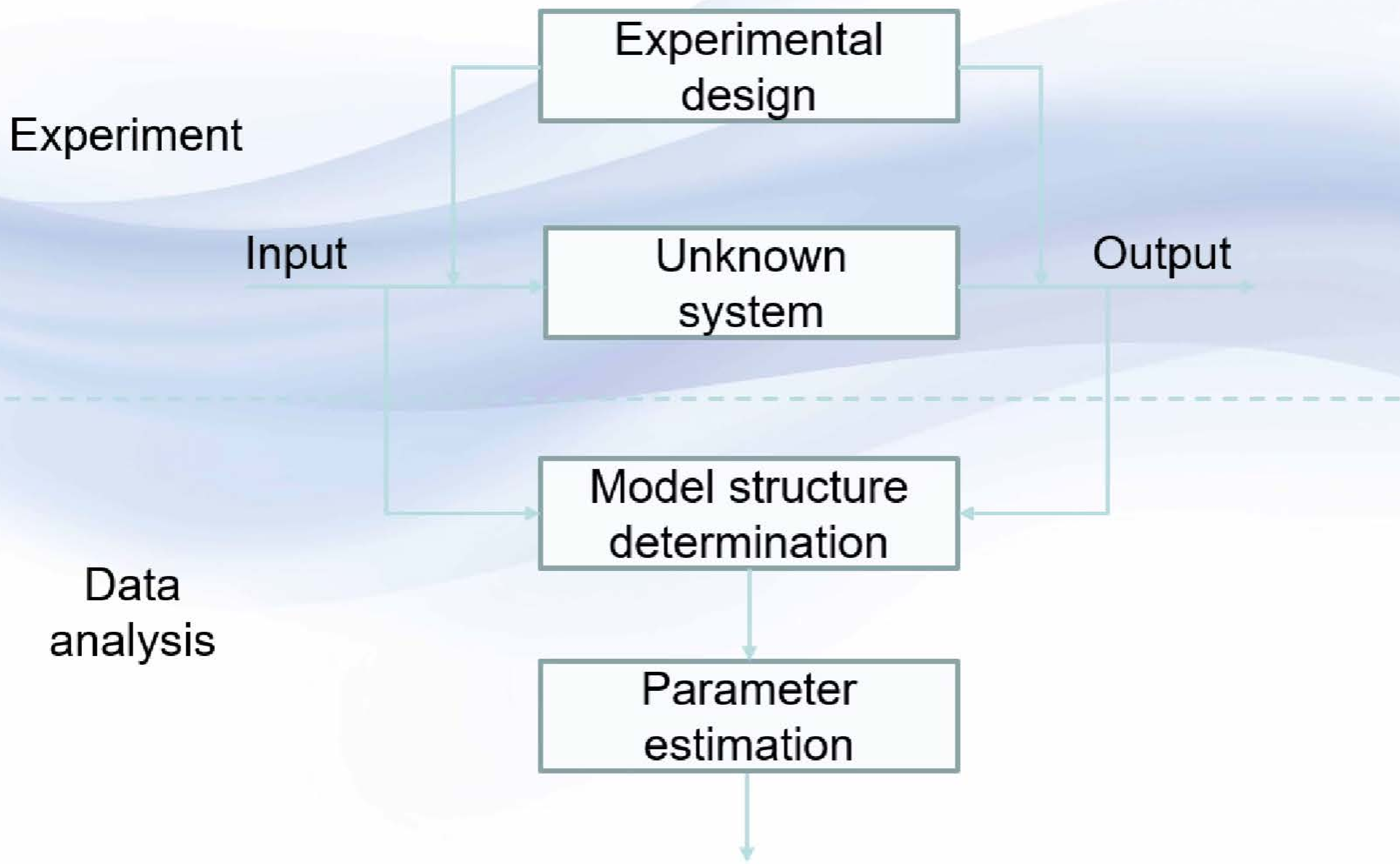
To complete the transformation from system to model, we must ***have both a model structure*** and **fully determined parameters corresponding to that structure**.

In other words, we need a <u>**complete model**</u>.

However, <u>we may not have such a model</u>.

We should by this stage have *at least one candidate model*, and we may have more than one to choose from.

Model identification



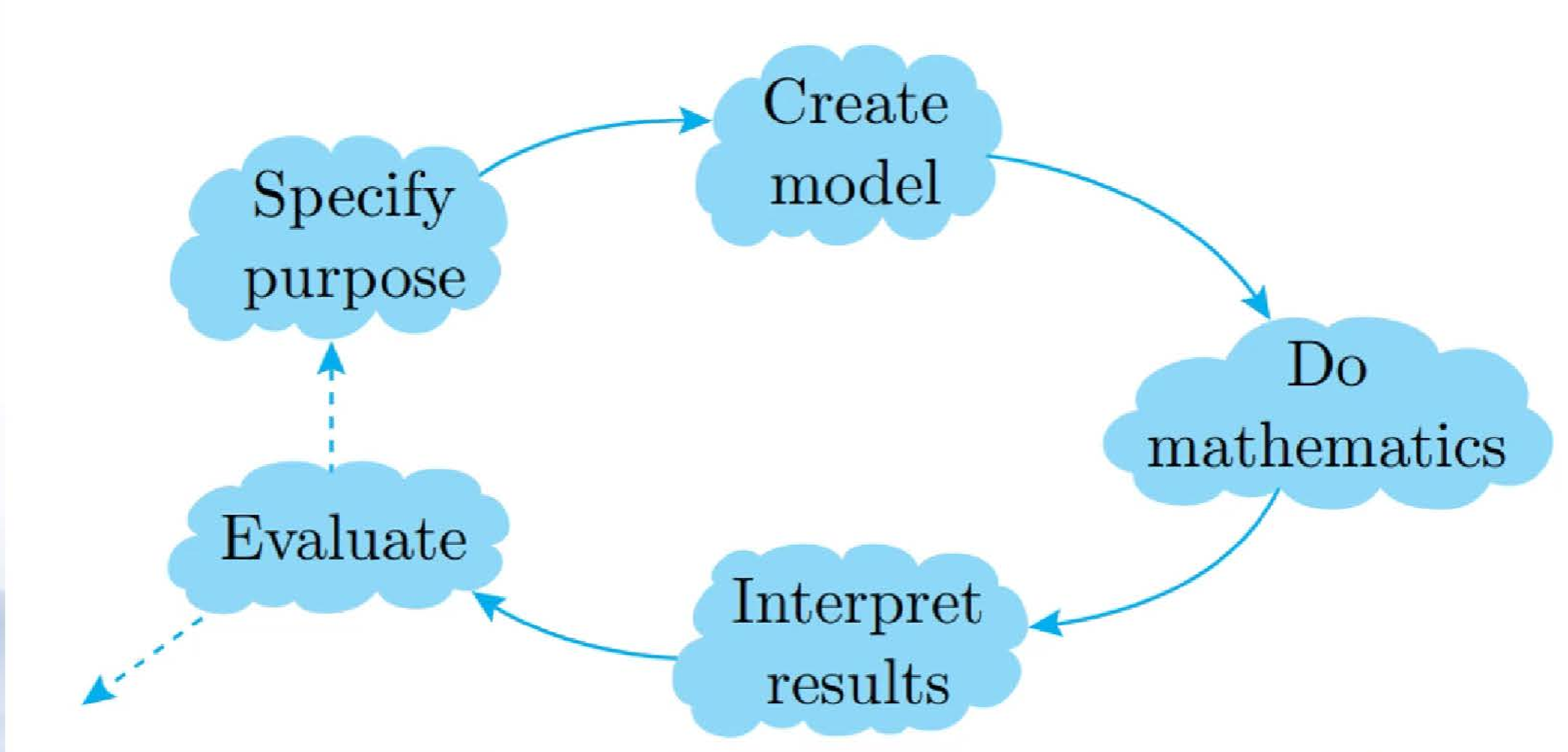
MODEL IDENTIFICATION

- In the identification process, data are mapped into parameter values by the model, where ***errors can occur in both the data and the model:***

-The first arises as a consequence of ***measurement errors***.

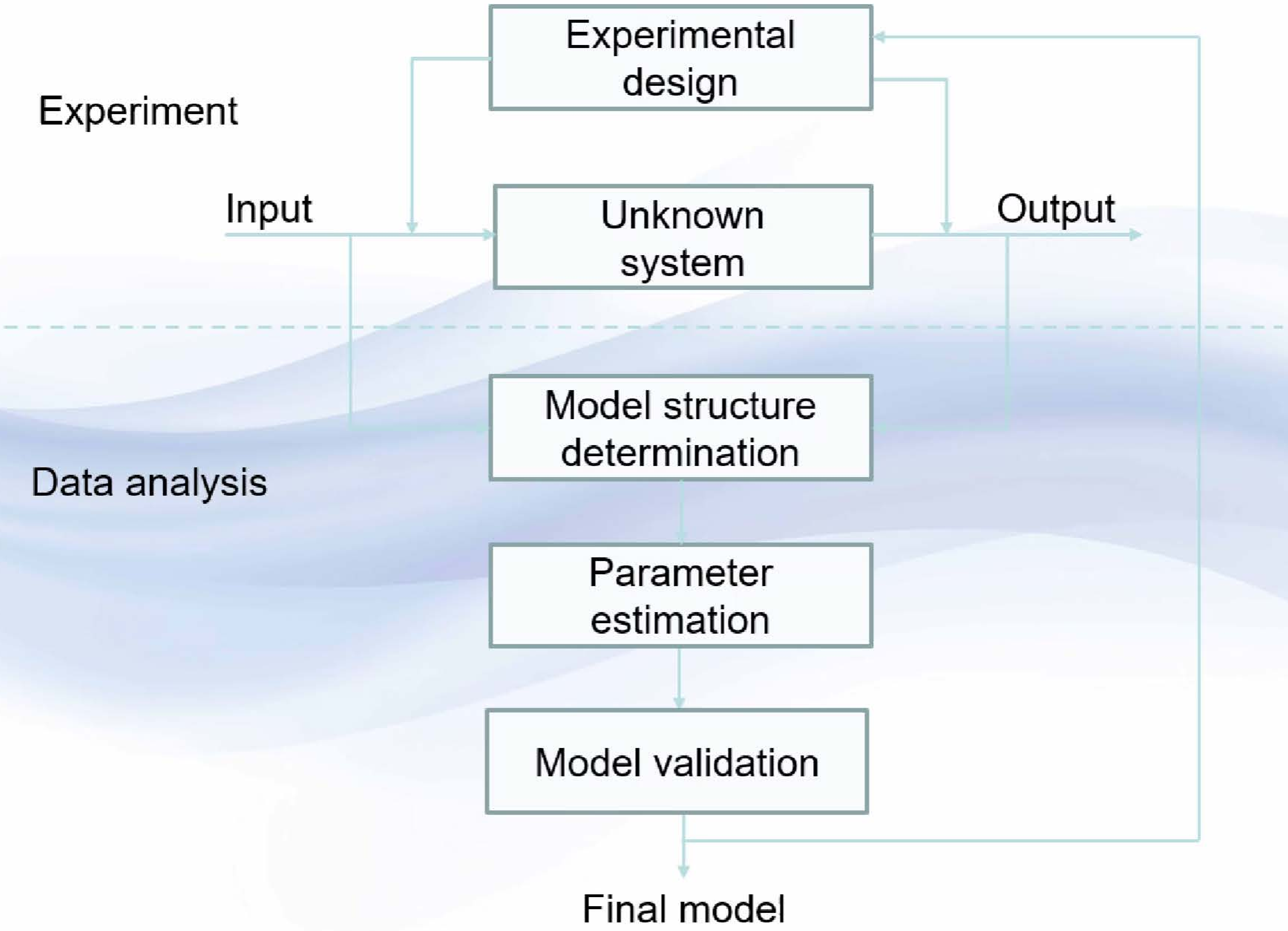
- The second involves ***errors in model structure***, which arise as a consequence of more than one competing model.

The evaluation of model performance

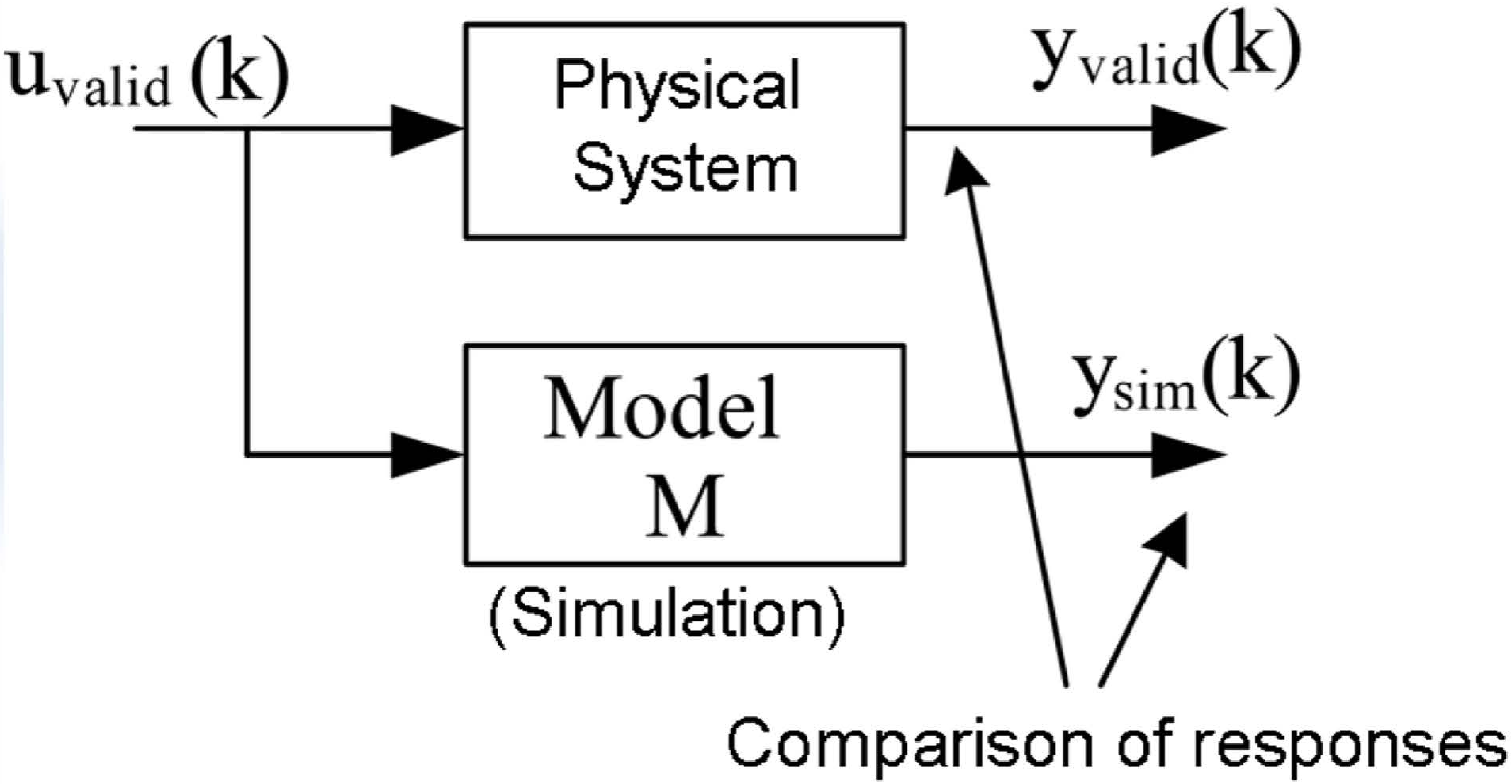


When evaluating a model, one *may find that it is not satisfactory for its purpose*.
Its *deficiencies must be identified* and an attempt to include additional features will follow.
That will lead to the **next pass** through the *modelling loop*.

Validation of the complete model

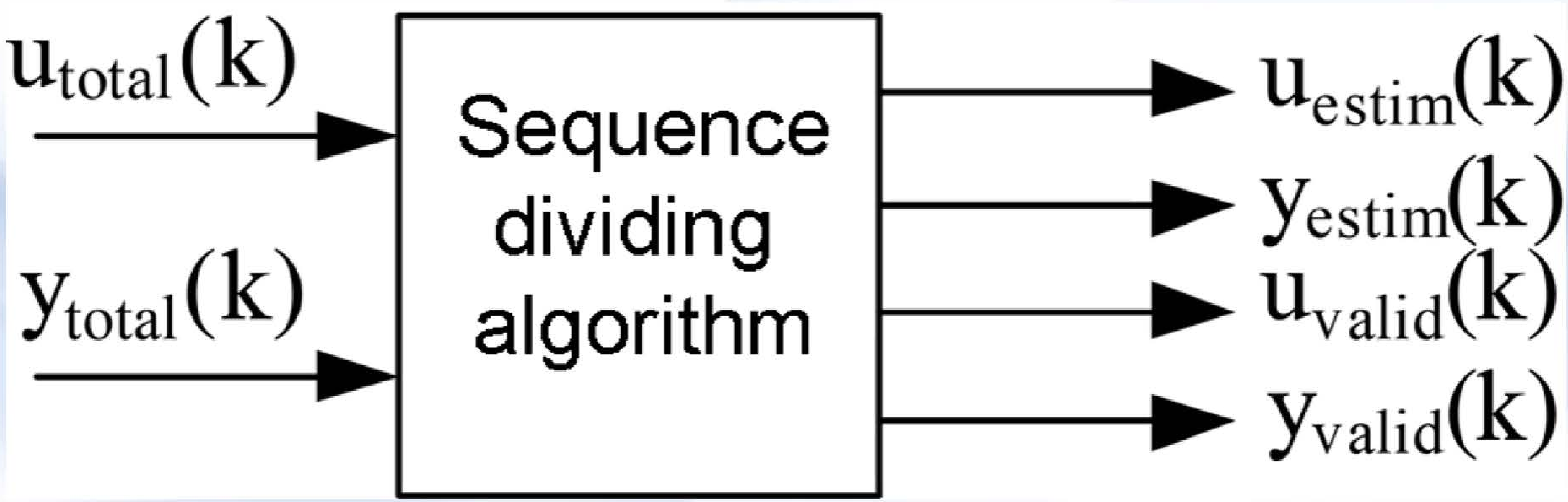


VALIDATION



$u_{valid}(k)$
Physical System
$y_{valid}(k)$
Model M
(Simulation)
$y_{sim}(k)$
Comparison of responses

VALIDATION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$y_{total}(k)$
Sequence dividing algorithm
$u_{estim}(k)$
$y_{estim}(k)$
$u_{valid}(k)$
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